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NEWS	3	NOV 26	MARPAT enhanced with FSORT command
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NEWS IPC8	For general information regarding STN implementation of IPC 8

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FILE 'HOME' ENTERED AT 07:49:24 ON 20 JAN 2009

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COST IN U.S. DOLLARS SINCE FILE TOTAL

	ENTRY	SESSION
FULL ESTIMATED COST	0.22	0.22

FILE 'REGISTRY' ENTERED AT 07:49:41 ON 20 JAN 2009

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 19 JAN 2009 HIGHEST RN 1094210-83-9
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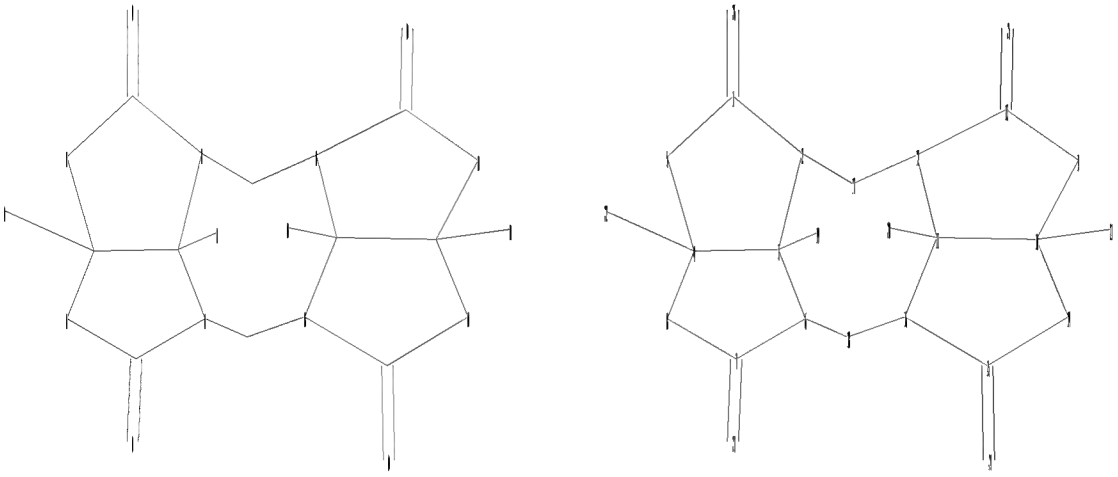

chain nodes :
19 20 21 22 23 24 25 26
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18
chain bonds :
1-26 3-19 4-22 7-23 10-21 11-20 13-25 15-24
ring bonds :
1-2 1-5 2-3 2-17 3-4 3-6 4-5 4-8 6-7 6-18 7-8 9-10 9-13 10-11 10-14 11-12 11-16 12-13 12-17 14-15 15-16 16-18

exact/norm bonds :
1-2 1-5 1-26 2-3 2-17 3-4 3-6 3-19 4-5 4-8 4-22 6-7 6-18 7-8 7-23
9-10 9-13 10-11 10-14 11-12 11-16 12-13 12-17 13-25 14-15 15-16 15-24
16-18
exact bonds :
10-21 11-20

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS
20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS

L1 STRUCTURE UPLOADED

=> d
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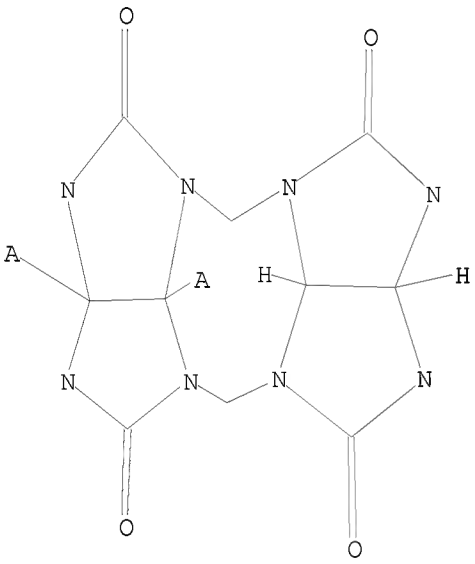
L1 STR



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SAMPLE SCREEN SEARCH COMPLETED - 216 TO ITERATE

100.0% PROCESSED 216 ITERATIONS 3 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 3439 TO 5201

PROJECTED ANSWERS: 3 TO 163

L2 3 SEA SSS SAM L1

=> l1 full
FULL SEARCH INITIATED 07:50:00 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 4159 TO ITERATE

100.0% PROCESSED 4159 ITERATIONS 35 ANSWERS
SEARCH TIME: 00.00.01

L3 35 SEA SSS FUL L1

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COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 185.88 186.10

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FILE LAST UPDATED: 19 Jan 2009 (20090119/ED)

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=> l3
L4 18 L3

=> d ibib abs hitstr 1-18

L4 ANSWER 1 OF 18 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2008:1372317 CAPLUS
DOCUMENT NUMBER: 150:55645
TITLE: Host-guest inclusion complexes of four partial alkyl-substituted cucurbit[6]urils with some probe guests
AUTHOR(S): Yu, Da-Hai; Ni, Xin-Long; Tian, Zhong-Cheng; Zhang,

Yun-Qin; Xue, Sai-Feng; Tao, Zhu; Zhu, Qing-Jiang
CORPORATE SOURCE: Key Laboratory of Macrocyclic and Supramolecular Chemistry of Guizhou Province, Guizhou University, Guiyang, 550025, Peop. Rep. China
SOURCE: Journal of Molecular Structure (2008), 891(1-3), 247-253
CODEN: JMOSB4; ISSN: 0022-2860
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Using probe guests, three host-guest inclusion complexes of two new alkyl-substituted cucurbit[6]uril hosts, ortho-tetramethyl cucurbit[6]uril (o-TMeQ[6]) and sym. tetracyclohexano cucurbit[6]uril (TCyHQ[6]) have been characterized successfully by single crystal X-ray diffractions. They are {o-TMeQ[6]-5,5'dimethyl-2,2'-bispyridine (DMBPY.H)+}Cl-21H2O(1), {(o-TMeQ[6])2-1,6-bisbenzoimidazolylhexane (SBH.2H)2+} 2Cl-52H2O (2) and {TCyHQ[6]-dioxane}14H2O (3). Moreover, two similar crystal structure of two inclusion complexes of other two partial substituted cucurbit[6]urils, meta-hexamethyl cucurbit[6]uril (m-HMeQ[6]) and sym. dicyclohexano cucurbit[6]uril (p-(CyH)2Q[6]) with HCl salt of DMBPY were also reported. They were {p-(CyH)2Q[6]-DMBPY +}Cl-16H2O (4) and {m-HMeQ[6]-DMBPY +}Cl-15H2O (5). The driving force for the information of the host-guest inclusion complexes can be attributed to not only the cavity interaction (host), but also the hydrogen bonding and ion-dipole interaction between the carbonyl oxygen at the portals of the host and the protonated nitrogen of the guest.
IT 1092792-08-9P 1092792-09-0P 1092792-10-3P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(crystallog.; host-guest inclusion complexes of four partial alkyl-substituted cucurbit[6]urils with some probe guests)
RN 1092792-08-9 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

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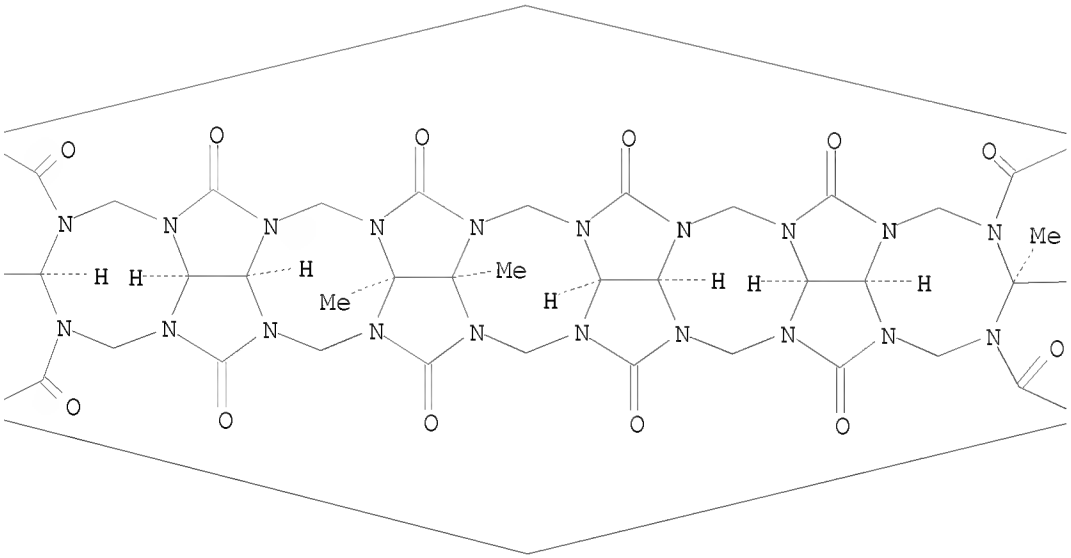
CRN 848440-56-2
CMF C40 H44 N24 O12

Relative stereochemistry.

PAGE 1-A

PAGE 1-B



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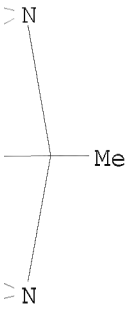

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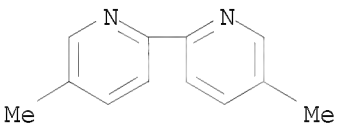

RN 1092792-09-0 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

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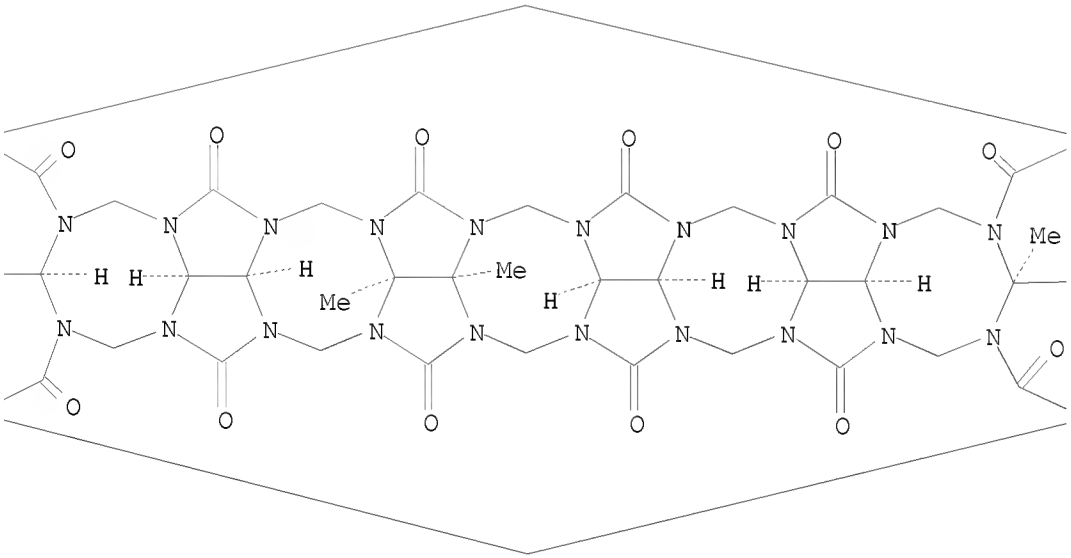
CRN 848440-56-2
CMF C40 H44 N24 O12

Relative stereochemistry.

PAGE 1-A

PAGE 1-B



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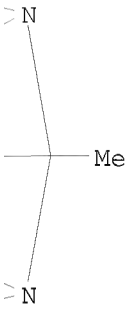

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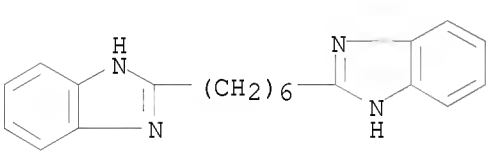

RN 1092792-10-3 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

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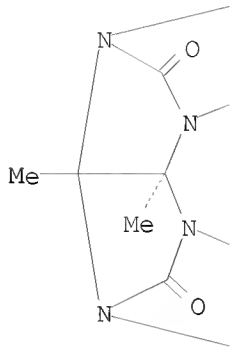
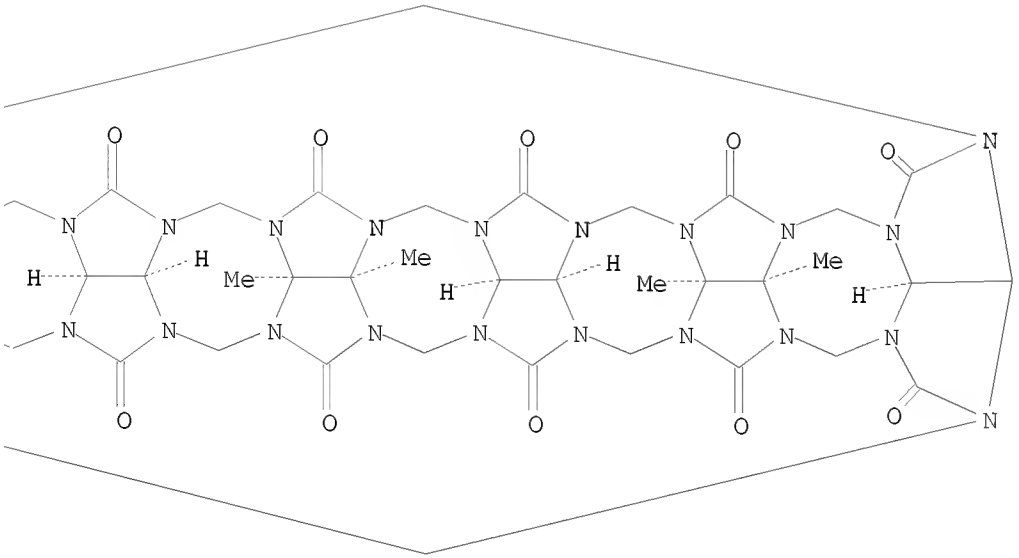
CRN 640732-36-1
CMF C42 H48 N24 O12

Relative stereochemistry.

PAGE 1-A



PAGE 1-B



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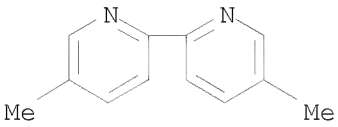
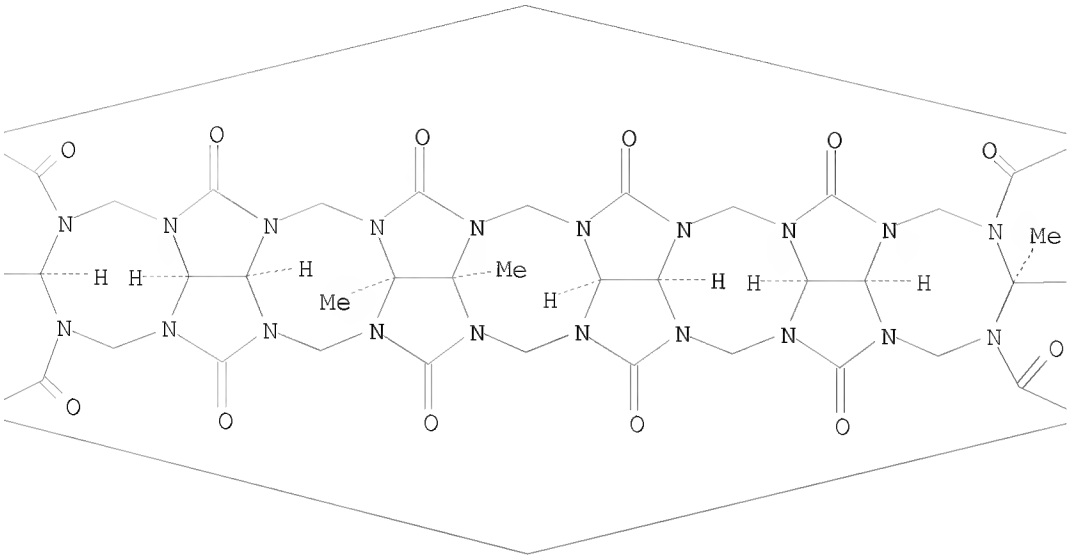


IT 848440-56-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(host, inclusion reaction; host-guest inclusion complexes of four partial alkyl-substituted cucurbit[6]urils with some probe guests)
RN 848440-56-2 CAPLUS
CN 1H,4H,14H,17H-2,16:3,15-Dimethano-5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-1,4,6,8,10,12,14,17,19,21,23,25-dodecone, dodecahydro-2a,21b,21c,26b-tetramethyl-, stereoisomer (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A

PAGE 1-B



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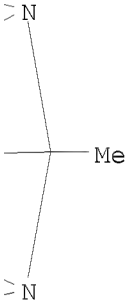

REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 18 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2008:1198526 CAPLUS
DOCUMENT NUMBER: 149:493259
TITLE: Interaction models of three alkyl substituted cucurbit[6]urils with a hydrochloride salt of 4,4'-dipyridyl guest
AUTHOR(S): Tian, Zhong-Cheng; Ni, Xin-Long; Xiao, Xin; Wu, Feng; Zhang, Yun-Qian; Zhu, Qian-Jiang; Xue, Sai-Feng; Tao,

Zhu
CORPORATE SOURCE: Key Laboratory of Macrocyclic and Supramolecular Chemistry of Guizhou Province, Guizhou University, Guiyang, 550025, Peop. Rep. China
SOURCE: Journal of Molecular Structure (2008), 888(1-3), 48-54
CODEN: JMOSB4; ISSN: 0022-2860
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Three host-guest complexes, {(H2O)2@(CyH)2Q[6]} (4,4'-bpyH)+·Cl-·10H2O (1), {(1,4-dioxane)@m-TriCyHQ[6]}(4,4'-bpyH)+·Cl-·19H2O (2), {(4,4'-bpyH2)2+@TMeQ[6]}.cntdot.2Br-.cntdot.11H2O (3), were prepared with three different alkyl substituted cucurbit[6]urils, sym. dicyclohexanocucurbit[6]uril {(CyH)2Q[6]}, meta tricyclohexanocucurbit[6]uril (m-TriCyHQ[6]), sym. tetramethylcucurbit[6]uril (TMeQ[6]), and a HCl salt 4,4'-dipyridyl(4,4'-bpyHCl) or a HBr salt 4,4'-dipyridyl[4,4-bpy(HBr)2] guest. Their crystal structures characterized by single-crystal X-ray diffractions revealed that these hosts can form supramol. assemblies with the halogen hydride salts of the guest 4,4'-bpy through the ion-dipole interaction, hydrogen bonding, C-H···π or N-H···π interaction and π···π stacking. The substituted alkyl group could affect the interaction model and assembled characteristic of the host and the guest.
IT 1072627-22-5P
RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(crystallog.; interaction models of three alkyl substituted cucurbit[6]urils with hydrochloride salt of 4,4'-dipyridyl guest)
RN 1072627-22-5 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

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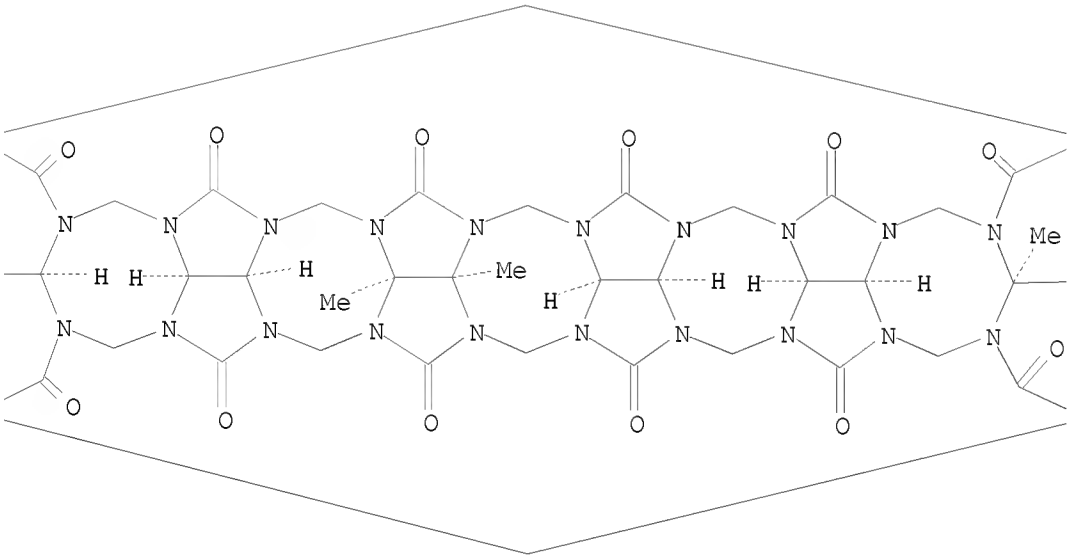
CRN 848440-56-2
CMF C40 H44 N24 O12

Relative stereochemistry.

PAGE 1-A

PAGE 1-B



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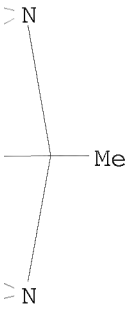

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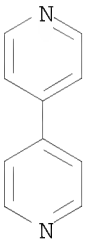

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L4 ANSWER 3 OF 18 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2008:928382 CAPLUS
DOCUMENT NUMBER: 149:322413
TITLE: Supramolecular Bracelets and Interlocking Rings Elaborated Through the Interrelationship of Neighboring Chemical Environments of Alkyl-Substitution on Cucurbit[5]uril
AUTHOR(S): Ni, Xin-Long; Lin, Jing-Xiang; Zheng, Yu-Ying; Wu, Wen-Shi; Zhang, Yun-Qian; Xue, Sai-Feng; Zhu, Qian-Jiang; Tao, Zhu; Day, Anthony I.
CORPORATE SOURCE: Key Laboratory of Macrocyclic and Supramolecular Chemistry of Guizhou Province, Guizhou University, Guiyang, Guizhou, 550025, Peop. Rep. China
SOURCE: Crystal Growth & Design (2008), 8(9), 3446-3450
CODEN: CGDEFU; ISSN: 1528-7483
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal
LANGUAGE: English

AB The smallest members of the cucurbituril family, cucurbit[5]uril (L1) and the alkyl-cucurbit[5]urils α,α'-dimethylcucurbit[5]uril (L2) and α,β,δ-tricyclohexanylcucurbit[5]uril (L3), can be used as a building blocks, linked by metal ions to create supramol. rings. Three supramol. complexes, {K2(H2O@L1)}[InCl4(H2O)2]·4.5H2O, {Sr2(Cl@L2)}Cl3·19H2O and {K3(H2O@L3)}Cl2·15.5H2O, were characterized by x-ray crystallog. The cavities found at the center of these rings have dimensions between 7 and 19 Å in width and 8.5 Å in depth. The partially substituted alkyl-cucurbit[5]urils present the most interesting supramol. ring formation. This occurs as a result of selective coordination of metal ions to the carbonyl oxygens of the glycoluril moieties carrying alkyl substitution.

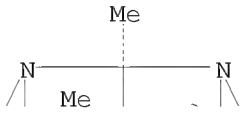
IT 569359-77-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of potassium aqua and strontium chloro supramol. complexes with cucurbit[5]uril and alkyl-cucurbit[5]urils)

RN 569359-77-9 CAPLUS

CN 1H,4H,12H,15H-2,14:3,13-Dimethano-5H,6H,7H,8H,9H,10H,11H,16H,17H,18H,19H,20H,21H,22H-2,3,4a,5a,6a,7a,8a,9a,10a,11a,13,14,15a,16a,17a,18a,19a,20a,21a,22a-eicosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-cd:1',2',3'-gh]pentalene-1,4,6,8,10,12,15,17,19,21-decone, decahydro-2a,22b-dimethyl-, stereoisomer (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



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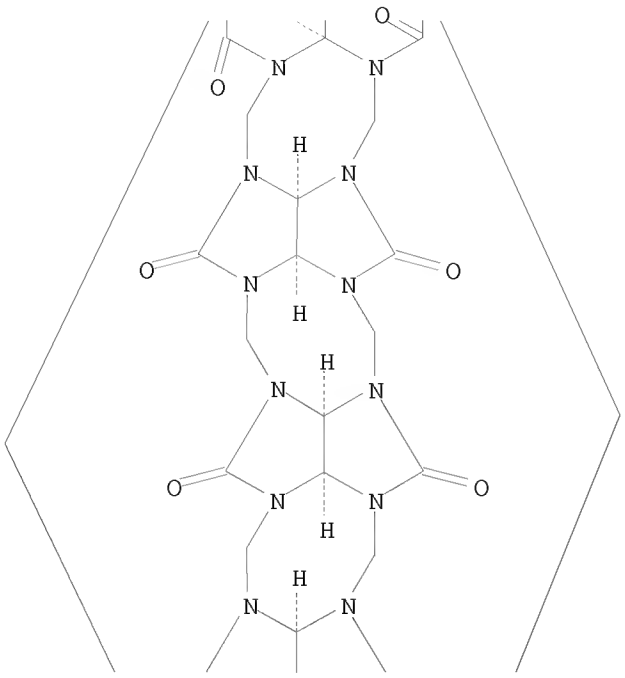
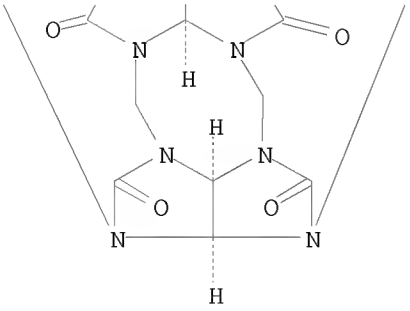


PAGE 3-A



REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 18 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2008:851115 CAPLUS
DOCUMENT NUMBER: 149:246169
TITLE: Supramolecular assemblies based on some new methyl-substituted cucurbit[5]urils through hydrogen bonding
AUTHOR(S): Lu, Li-Bin; Yu, Da-Hai; Zhang, Yun-Qian; Zhu, Qian-Jiang; Xue, Sai-Feng; Tao, Zhu
CORPORATE SOURCE: Key Laboratory of Macrocyclic and Supramolecular Chemistry of Guizhou Province, Guizhou University,

Guiyang, 550025, Peop. Rep. China
SOURCE: Journal of Molecular Structure (2008), 885(1-3), 70-75
CODEN: JMOSB4; ISSN: 0022-2860
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

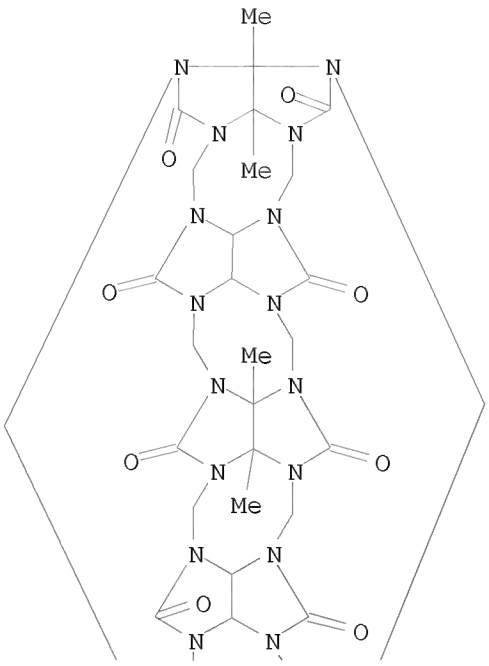
AB Three supramol. assemblies based on three new partial methyl-substituted cucurbit[5]urils, which are tetramethylcucurbit[5]uril (α,γ-TMeQ[5]), hexamethyl cucurbit[5]uril (α,β,δ-HMeQ[5]), nonamethylcucurbit[5]uril (NMeQ[5]), were synthesized and structurally characterized by single-crystal X-ray diffractions. For the comparison with these new Q[5]s, crystal structure of an assembly constructing with normal Q[5] and K2PtCl6 was also reported. They are (α,γ-TMeQ[5])·15(H2O) (1), (α,β,δ-HMeQ[5])·2Cl-·2(H3O)+·7(H2O) (2), (NMeQ[5])·14(H2O) (3), (Q[5])2·[K(H2O)]2+· [PtCl6]2-·24(H2O) (4). In the corresponding crystal structures, the mol. encapsulates included a water mol. and lidded water mols. at both of the portals were observed Moreover, these mol. encapsulates are connected through hydrogen bonding and formed supramol. chains or joined in pair.

IT 1045861-31-1P 1045861-33-3P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(crystallog.; H-bonded supramol. assemblies based on methyl-substituted cucurbit[5]urils)

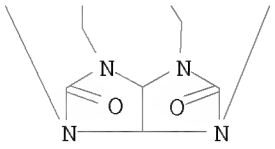
RN 1045861-31-1 CAPLUS

CN 1H,4H,12H,15H-2,14:3,13-Dimethano-5H,6H,7H,8H,9H,10H,11H,16H,17H,18H,19H,20H,21H,22H-2,3,4a,5a,6a,7a,8a,9a,10a,11a,13,14,15a,16a,17a,18a,19a,20a,21a,22a-eicosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-cd:1',2',3'-gh]pentalene-1,4,6,8,10,12,15,17,19,21-decone, decahydro-2a,19b,19c,22b-tetramethyl-, hydrate (1:15), stereoisomer (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



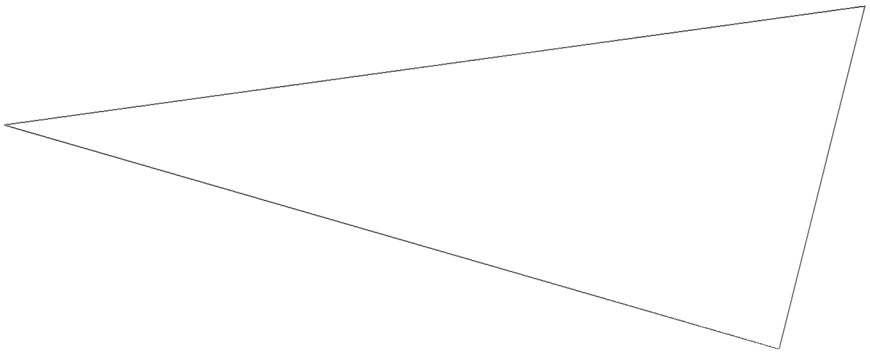
●15 H_2O

RN 1045861-33-3 CAPLUS
CN 1H,4H,12H,15H-2,14:3,13-Dimethano-
5H,6H,7H,8H,9H,10H,11H,16H,17H,18H,19H,20H,21H,22H-
2,3,4a,5a,6a,7a,8a,9a,10a,11a,13,14,15a,16a,17a,18a,19a,20a,21a,22a-
eicosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pe
ntaleno[1',6':5,6,7]cycloocta[1,2,3-cd:1',2',3'-gh]pentalene-
1,4,6,8,10,12,15,17,19,21-decone, decahydro-2a,17b,17c,21b,21c,22b-
hexamethyl-, hydrochloride, hydrate (1:2:9), stereoisomer (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A

PAGE 1-C



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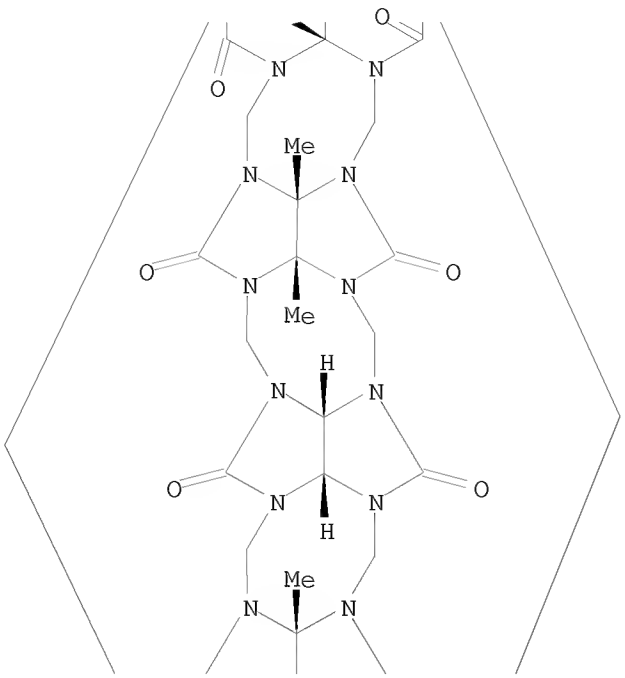
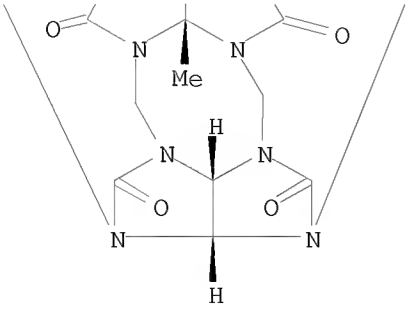


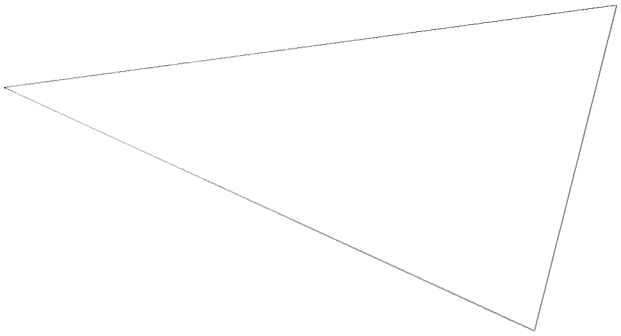
PAGE 3-A



● 2 HCl

● 9 H_2O

PAGE 3-C



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 18 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2008:668053 CAPLUS
DOCUMENT NUMBER: 149:214504
TITLE: Structures of supramolecular assemblies formed by some partial substituted cucurbiturils and some metal ion complexes
AUTHOR(S): Yu, Da-Hai; Ni, Xin-Long; Zhang, Yun-Qian; Xue, Sai-Feng; Zhu, Qian-Jiang; Tao, Zhu
CORPORATE SOURCE: Key Laboratory of Macrocyclic and Supramolecular Chemistry of Guizhou Province, Guizhou University, Guiyang, 550025, Peop. Rep. China
SOURCE: Journal of Molecular Structure (2008), 882(1-3), 128-133
CODEN: JMOSB4; ISSN: 0022-2860
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

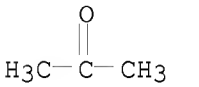
AB Three supramol. assemblies based on substituted cucurbit[6]uril, α,δ-tetramethylcucurbit[6]uril (TMeQ[6]), α,γ,ε-tricyclohexylcucurbit[6]uril (m-TriCyHQ[6]), and α,γ,ε-hexamethylcucurbit[6]uril (m-HMeQ[6]) with different metal ions were synthesized and structurally characterized by single-crystal x-ray diffractions. They are {TMeQ[6]@acetone[Ca(H2O)3]}2+·(CdCl4)2-·10H2O (1), {[m-TriCyHQ[6]@dioxane][Na(H2O)2Cl]}·15H2O (2) and {[m-HMeQ[6]]K2(H2O)4Cl}Cl·15H2O (3). The crystal structures of these complexes showed the different interaction modes between these partial alkyl-substituted cucurbit[6]urils and the metal ions. In compound 1, a 1-dimensional supramol. chain of alternating TMeQ[6] mols. and [Ca(H2O)3]2+ complexes assembled through coordination bonding of the cation and the carbonyl oxygens of TMeQ[6]. The compound 2 was the 1st reported crystal structure of the m-TriCyHQ[6] with metal ion through the coordinate bonds, and the compound 3 was the 1st reported crystal structure of m-HMeQ[6]. It was unexpected that an ionic bonded chloride anion was at the portal of the two meta-substituted cucurbiturils.

IT 1042142-05-1P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(one-dimensional chain polymer; preparation and crystal and mol. structure)

RN 1042142-05-1 CAPLUS
CN Calcium(2+), triaqua(dodecahydro-2a,21b,21c,26b-tetramethyl-1H,4H,14H,17H-2,16:3,15-dimethano-5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-1,4,6,8,10,12,14,17,19,21,23,25-dodecone-κO1,κO17)-, (T-4)-tetrachlorocadmate(2-), compd. with 2-propanone, hydrate (1:1:1:10) (CA INDEX NAME)

CM 1

CRN 67-64-1
CMF C3 H6 O



CM 2

CRN 1042142-04-0
CMF C40 H50 Ca N24 O15 . Cd Cl4

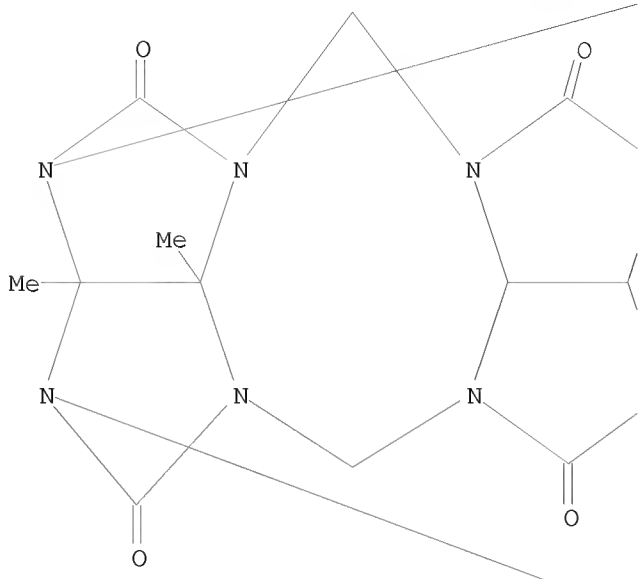
CM 3

CRN 1042142-03-9
CMF C40 H50 Ca N24 O15
CCI CCS

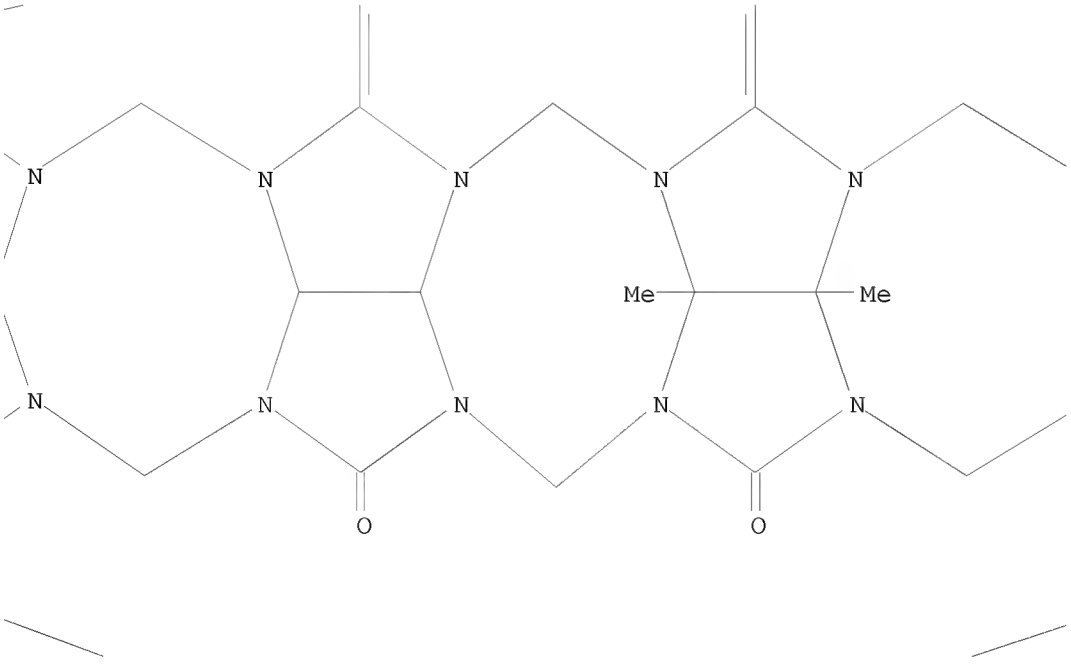
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

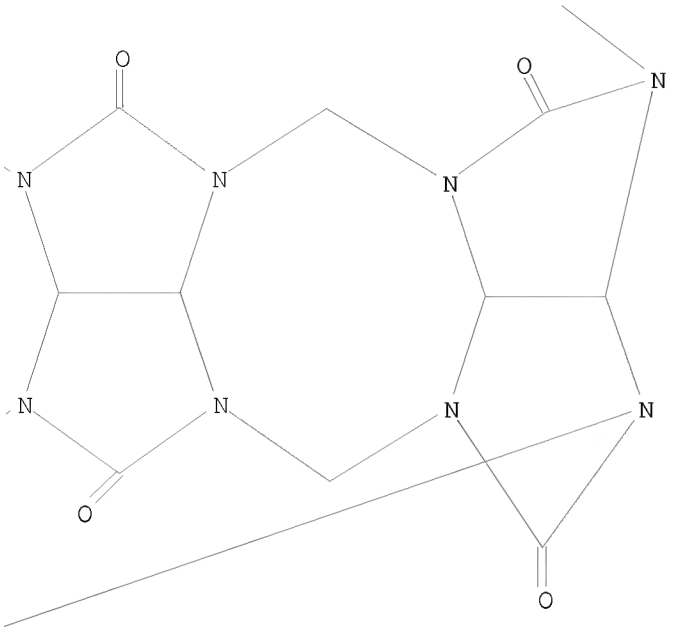
PAGE 2-A



PAGE 2-B



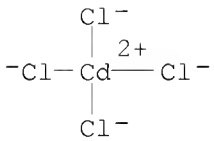
PAGE 2-C



PAGE 3-B

CM 4

CRN 15974-49-9
CMF Cd Cl4
CCI CCS

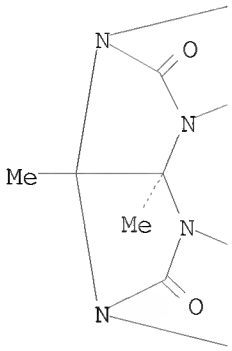


IT 640732-36-1 848440-56-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of calcium, sodium and potassium complexes with substituted cucurbit[6]urils)
RN 640732-36-1 CAPLUS

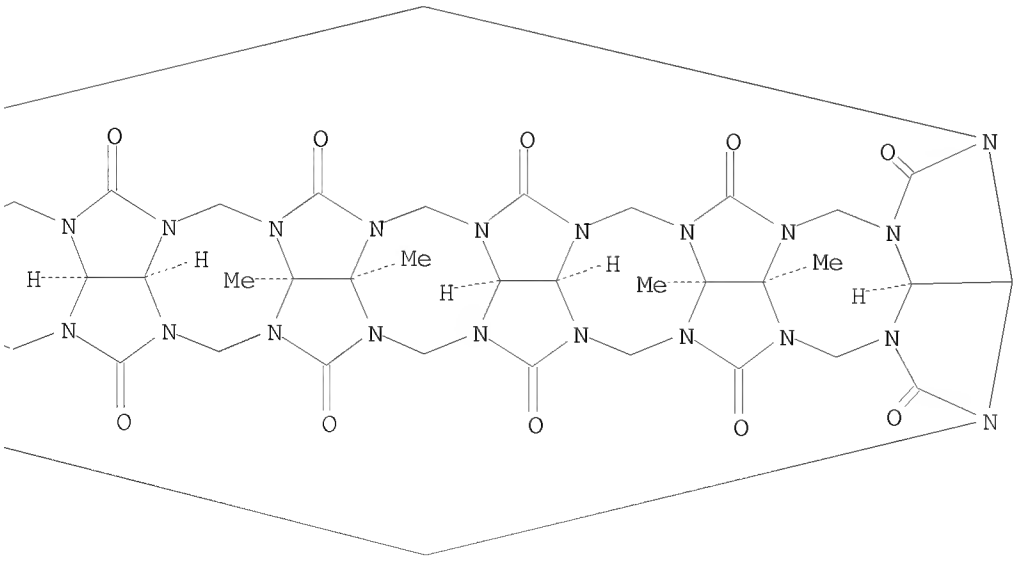
CN 1H,4H,14H,17H-2,16:3,15-Dimethano-
5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-
2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-
1,4,6,8,10,12,14,17,19,21,23,25-dodecone,
dodecahydro-2a,19b,19c,23b,23c,26b-hexamethyl-, stereoisomer (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



PAGE 1-B

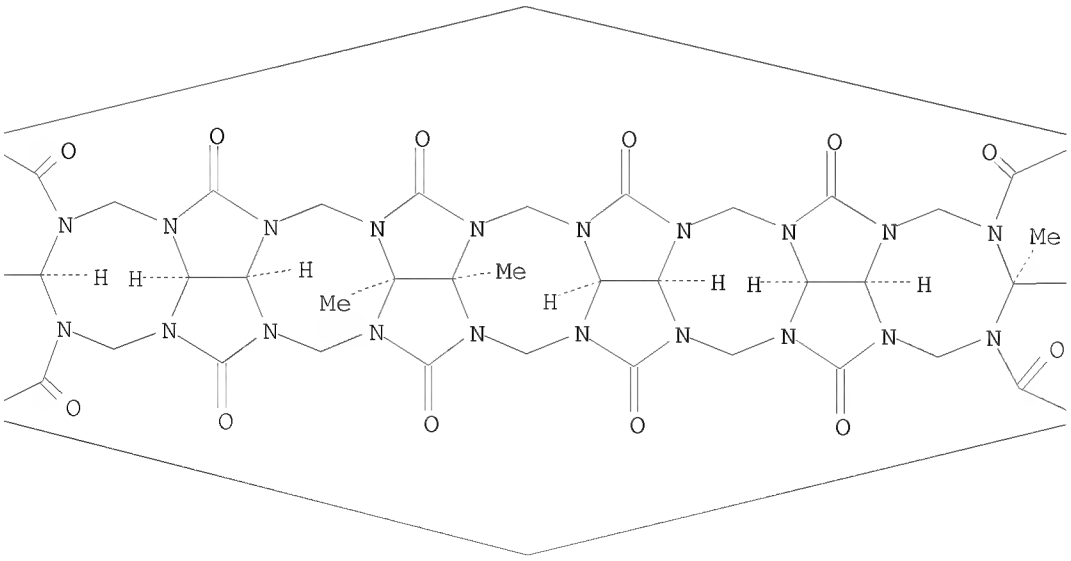


RN 848440-56-2 CAPLUS
CN 1H,4H,14H,17H-2,16:3,15-Dimethano-
5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-
2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-
1,4,6,8,10,12,14,17,19,21,23,25-dodecone,
dodecahydro-2a,21b,21c,26b-tetramethyl-, stereoisomer (CA INDEX NAME)

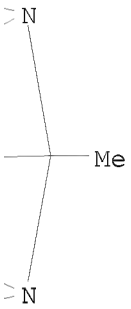
Relative stereochemistry.

PAGE 1-A

PAGE 1-B



PAGE 1-C



REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 18 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2008:272306 CAPLUS
DOCUMENT NUMBER: 148:508829
TITLE: Structures of supramolecular assemblies formed by substituted cucurbiturils and metal ions
AUTHOR(S): Zhang, Yun-Qian; Zhen, Li-Mei; Yu, Da-Hai; Zhao, Yun-Jie; Xue, Sai-Feng; Zhu, Qian-Jiang; Tao, Zhu
CORPORATE SOURCE: Institute of Applied Chemistry, Guizhou University, Guiyang, 550025, Peop. Rep. China
SOURCE: Journal of Molecular Structure (2008), 875(1-3), 435-441
CODEN: JMOSB4; ISSN: 0022-2860
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 148:508829
AB Four supramol. assemblies based on two partial substituted cucurbituril, α,δ-tetramethylcucurbit[6]uril (TMeQ[6]) and α,δ-dicyclohexanocucurbit[6]uril ((CyH)2Q[6]), with different metal ions were synthesized and structurally characterized by single-crystal x-ray diffractions. They are {[TMeQ[6]@2H2O].cntdot.[Zn(H2O)4]}·[ZnCl4]·12H2O (1), {[TMeQ[6]@H2O].cntdot.[Sr2Cl2]}.cntdot.[Cl]2.cntdot.10H2O (2), {TMeQ[6]·[CaCl]}·[Cl]·17.5H2O (3), {[(CyH)2Q[6]@acetone].cntdot.1.5[Ni(H2O)6]}·(NO3)32H2O (4). The crystal structures of these complexes showed that supramol. chains were formed through different interaction modes. In complex 1, the transition metal ion Zn2+ was coordinated not only with H2O mols. but also directly with carbonyl oxygens of a portal of TMeQ[6]. The Zn aqua complexes served as a bridge between TMeQ[6]s in the 1-dimensional supramol. chains. In complex 2, each Sr2+ ion was coordinated directly with two carbonyl O atoms at a portal of two TMeQ[6], and each TMeQ[6] was coordinated with

four Sr2+ ions, giving supramol. chains consisted of alternating metal ions and TMeQ[6]. In 3, two TMeQ[6] mols. were coordinated by two Ca2+ ions to form a assembled unit. The assembled units were connected through H bonds, giving supramol. chains. In complex 4, supramol. chains consisted of alternating [Ni(H2O)]2+ complex cation and (CyH)2Q[6] were formed through H bonding.

IT 848440-56-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(for preparation of zinc, strontium, calcium and nickel complexes with substituted cucurbiturils)

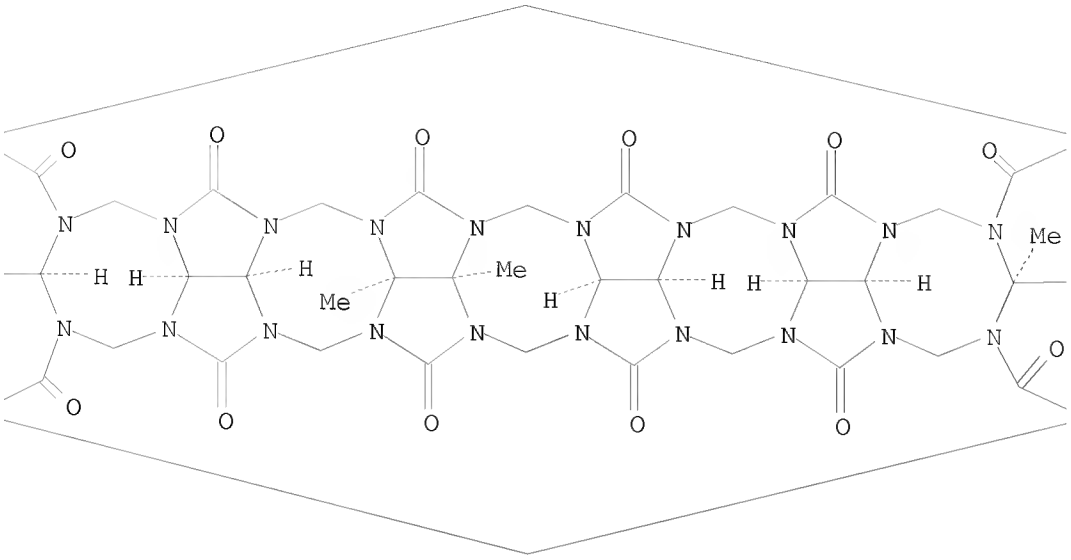
RN 848440-56-2 CAPLUS

CN 1H,4H,14H,17H-2,16:3,15-Dimethano-5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-1,4,6,8,10,12,14,17,19,21,23,25-dodecone, dodecahydro-2a,21b,21c,26b-tetramethyl-, stereoisomer (CA INDEX NAME)

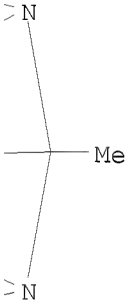
Relative stereochemistry.

PAGE 1-A

PAGE 1-B



PAGE 1-C



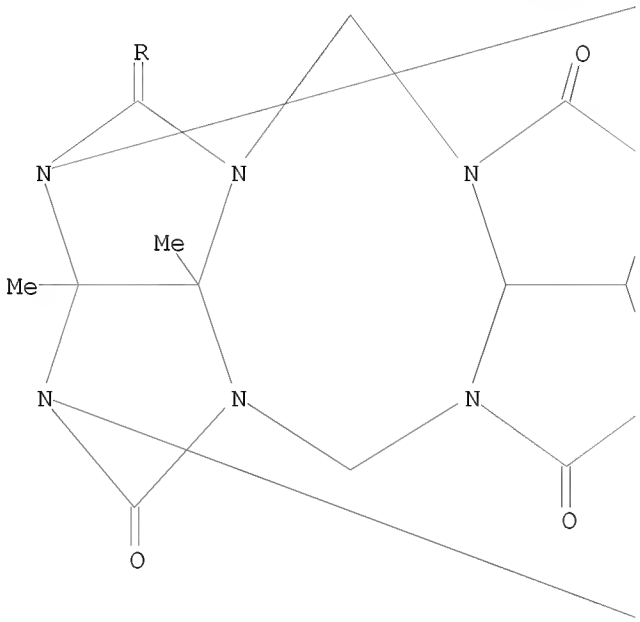
IT 1020725-95-4P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(polymeric; preparation and crystal structure of supramol. complex)
RN 1020725-95-4 CAPLUS
CN Strontium, hexaaquatetrachloro[μ-(dodecahydro-2a,21b,21c,26b-tetramethyl-1H,4H,14H,17H-2,16:3,15-dimethano-5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-

1,4,6,8,10,12,14,17,19,21,23,25-dodecone-
κO1,κO17:κO21)]di-, hydrate (1:14) (CA INDEX NAME)

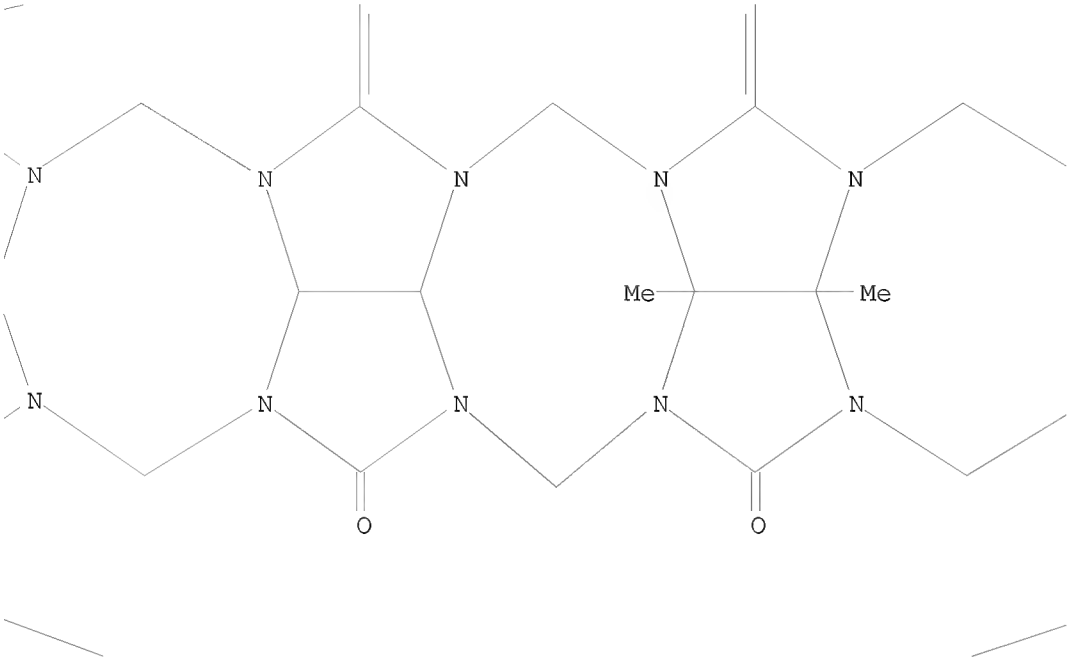
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

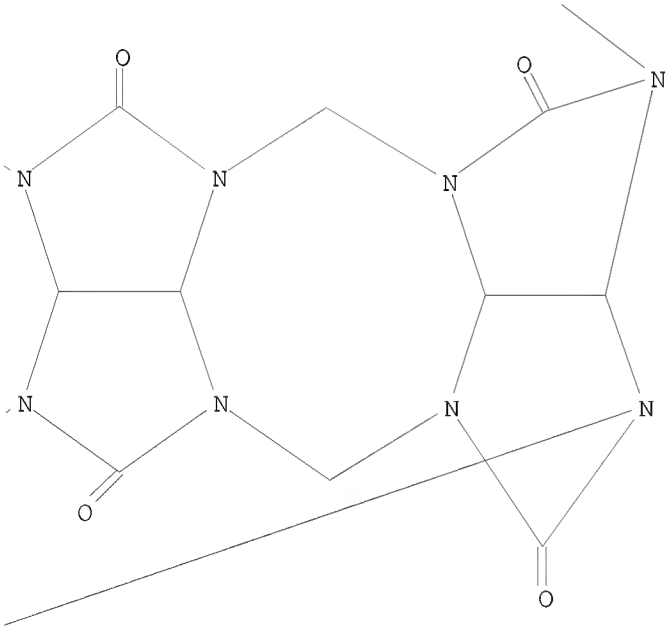
PAGE 2-A



PAGE 2-B



PAGE 2-C



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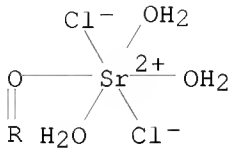


●14 H_2O

PAGE 3-B

IT 1020725-94-3P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal structure of supramol. complex)
RN 1020725-94-3 CAPLUS
CN Zinc(2+), tetraaqua(dodecahydro-2a,21b,21c,26b-tetramethyl-1H,4H,14H,17H-2,16:3,15-dimethano-5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-1,4,6,8,10,12,14,17,19,21,23,25-dodecone-κO1,κO17)-, (OC-6-22)-, (T-4)-tetrachlorozincate(2-), hydrate (1:1:14) (CA INDEX NAME)

CM 1

CRN 1020725-93-2
CMF C40 H52 N24 O16 Zn . Cl4 Zn

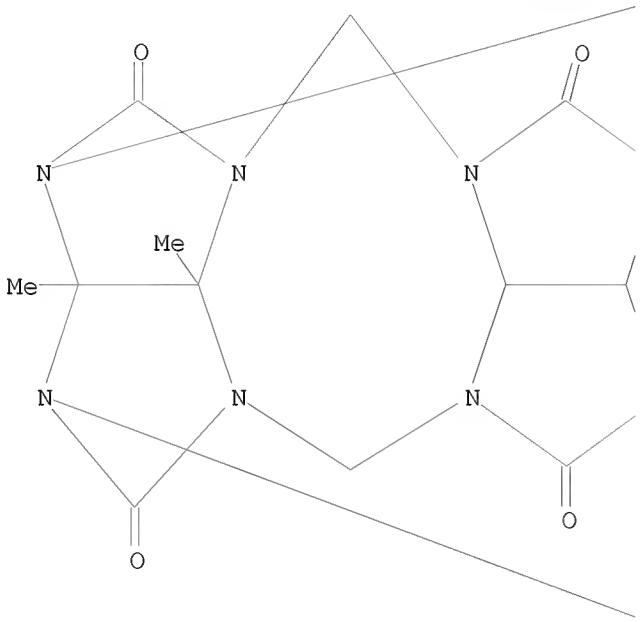
CM 2

CRN 1020725-92-1
CMF C40 H52 N24 O16 Zn
CCI CCS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

PAGE 2-A



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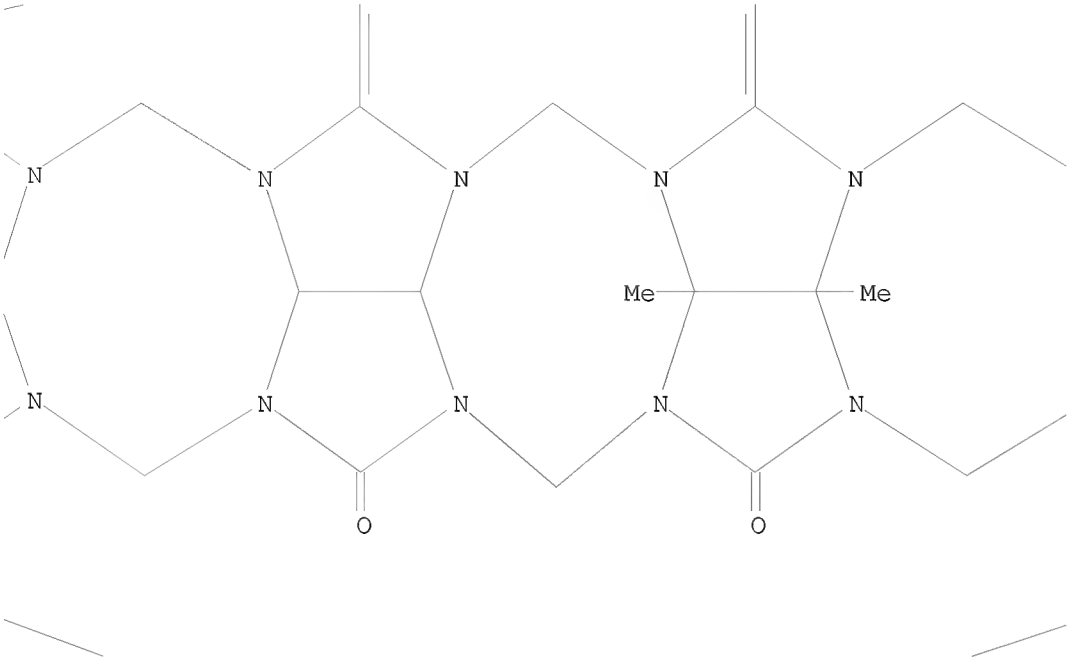

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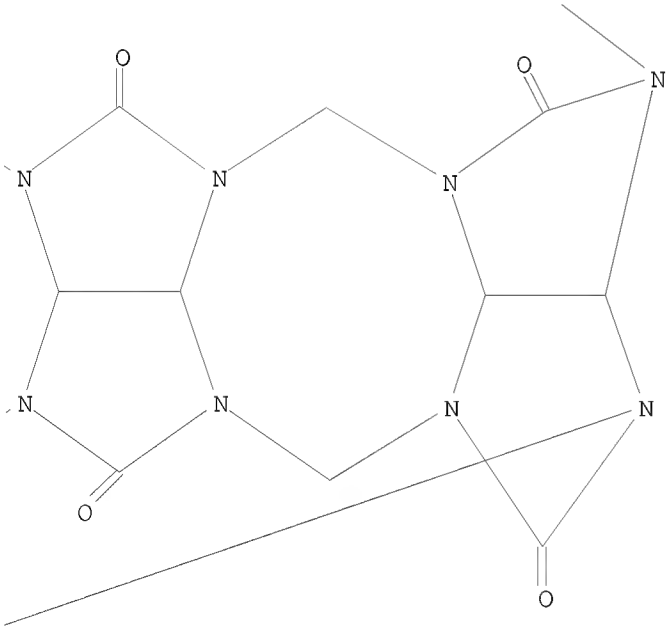
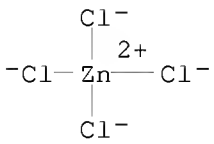


PAGE 3-B

CM 3

CRN 15201-05-5
CMF Cl4 Zn
CCI CCS



REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 18 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2008:111164 CAPLUS
DOCUMENT NUMBER: 148:262631
TITLE: Method for synthesis of cucurbit[n]urils and substituted cucurbit[n]urils compounds
INVENTOR(S): Xue, Saifeng; Zhu, Qianjiang; Tao, Zhu
PATENT ASSIGNEE(S): Guizhou University, Peop. Rep. China
SOURCE: Faming Zhuanli Shenqing Gongkai Shuomingshu, 10pp.
CODEN: CNXXEV
DOCUMENT TYPE: Patent
LANGUAGE: Chinese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CN 101108851	A	20080123	CN 2007-10077837	20070711

PRIORITY APPLN. INFO.: CN 2007-10077837 20070711

AB The method comprises react glycoluril dimer with an epoxy glycoluril or an epoxy glycoluril derivative and formaldehyde in ratio 1:0-4:0-4 in hydrochloric acid at 90-100° for 1-2 h, concentrating, filtrating, separating and purifying to form cucurbit[n]urils or substituted cucurbit[n]urils, wherein the content of epoxy glycoluril or its derivative and formaldehyde is not simultaneously 0. The formaldehyde can be replaced by hexamethylenetetramine or polyformaldehyde; HCl can be replaced by sulfuric acid. With the method, the distribution of cucurbit[n]urils in product and the amount and position of substations groups in cucurbit[n]urils can be easily controlled.

IT 848440-56-2P

RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(method for synthesis of cucurbit[n]urils and substituted cucurbit[n]urils compds.)

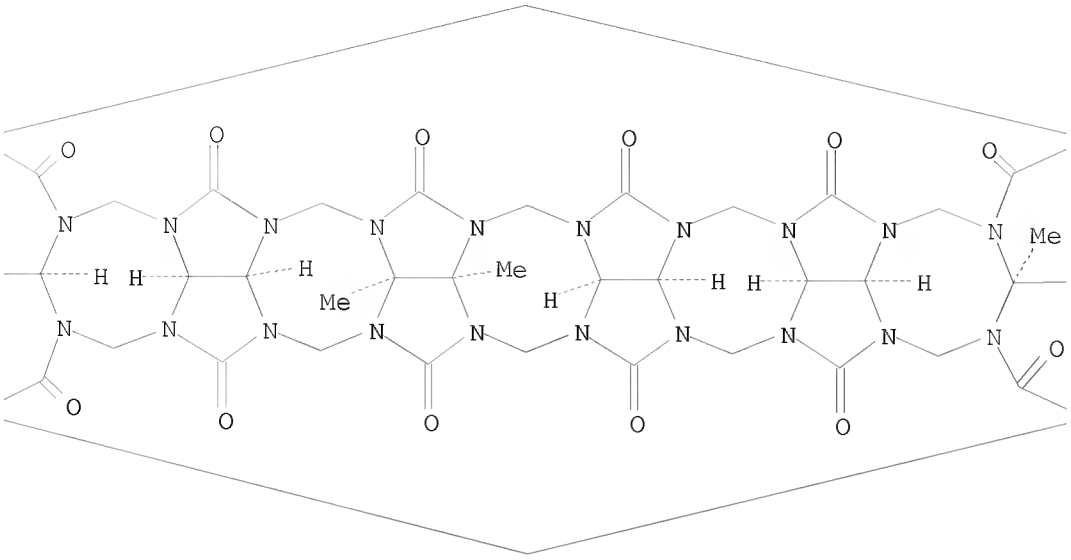
RN 848440-56-2 CAPLUS

CN 1H,4H,14H,17H-2,16:3,15-Dimethano-5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-1,4,6,8,10,12,14,17,19,21,23,25-dodecone, dodecahydro-2a,21b,21c,26b-tetramethyl-, stereoisomer (CA INDEX NAME)

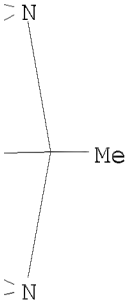
Relative stereochemistry.

PAGE 1-A

PAGE 1-B



PAGE 1-C



L4 ANSWER 8 OF 18 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2007:1339803 CAPLUS
DOCUMENT NUMBER: 148:561422
TITLE: Studies of the interaction of tetramethylcucurbit[6]uril and 5,5'-dimethyl-2,2'-bipyridyl hydrochloride
AUTHOR(S): Cong, Hang; Zhao, Yun-Jie; Xue, Sai-Feng; Tao, Zhu; Zhu, Qian-Jiang
CORPORATE SOURCE: Institute of Applied Chemistry, Guizhou University, Guiyang, 550025, Peop. Rep. China

SOURCE: Journal of Molecular Modeling (2007), 13(12), 1221-1226
CODEN: JMMOFK; ISSN: 0948-5023
URL: http://www.springerlink.com/content/x6nw1j3949222664/fulltext.pdf
PUBLISHER: Springer GmbH
DOCUMENT TYPE: Journal; (online computer file)
LANGUAGE: English

AB The interaction between tetramethylcucurbit[6]uril (host) and 5,5'-dimethyl-2,2'-bipyridyl hydrochloride (guest) was studied by 1H NMR, x-ray crystallog., electronic absorption spectroscopy, fluorescence emission spectra and quantum chemical calcns. This exptl.-computational study that indicated the host can orientationally encapsulate the guest with a moderate association constant value. Computation qual. explained the split UV-visible absorption peak of the inclusion complex.

IT 1026700-36-6
RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); FORM (Formation, nonpreparative); PROC (Process)
(interaction of tetramethylcucurbit[6]uril host and 5,5'-dimethyl-2,2'-bipyridyl hydrochloride guest)

RN 1026700-36-6 CAPLUS

CN 1H,4H,14H,17H-2,16:3,15-Dimethano-5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-1,4,6,8,10,12,14,17,19,21,23,25-dodecone, dodecahydro-2a,21b,21c,26b-tetramethyl-, stereoisomer, compd. with 5,5'-dimethyl-2,2'-bipyridine hydrochloride, hydrate (1:1:1:?) (CA INDEX NAME)

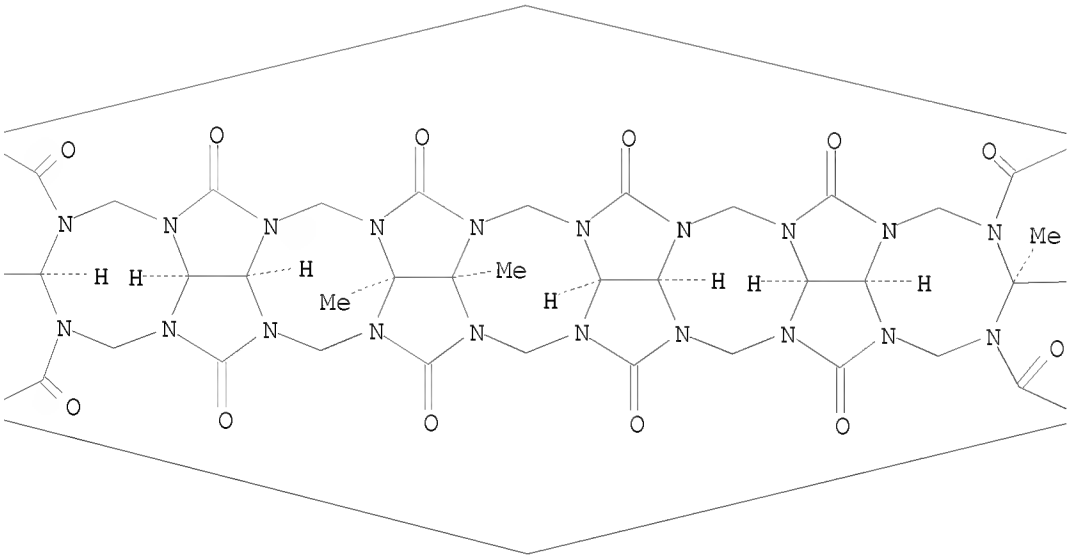
CM 1

CRN 848440-56-2
CMF C40 H44 N24 O12

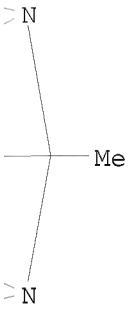
Relative stereochemistry.

PAGE 1-A

PAGE 1-B

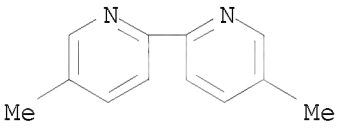


PAGE 1-C



CM 2

CRN 1762-34-1
CMF C12 H12 N2

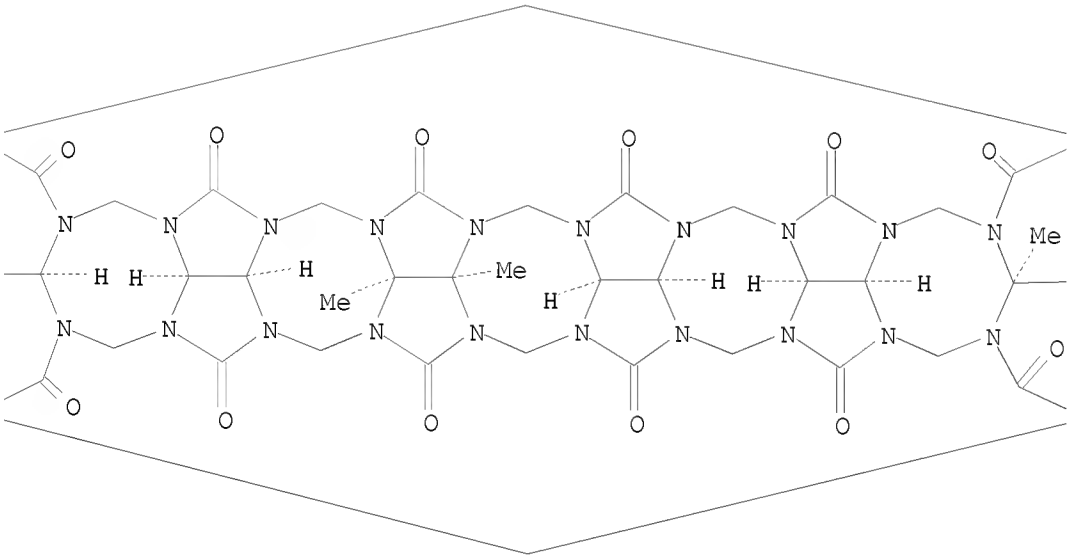


IT 848440-56-2
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(interaction of tetramethylcucurbit[6]uril host and
5,5'-dimethyl-2,2'-bipyridyl hydrochloride guest)
RN 848440-56-2 CAPLUS
CN 1H,4H,14H,17H-2,16:3,15-Dimethano-
5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-
2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-
1,4,6,8,10,12,14,17,19,21,23,25-dodecone,
dodecahydro-2a,21b,21c,26b-tetramethyl-, stereoisomer (CA INDEX NAME)

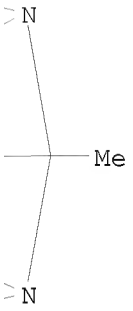
Relative stereochemistry.

PAGE 1-A

PAGE 1-B



PAGE 1-C



REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 18 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2007:508326 CAPLUS
DOCUMENT NUMBER: 147:165907
TITLE: Synthesis and X-ray structure of the inclusion complex of dodecamethylcucurbit[6]uril with 1,4-dihydroxybenzene
AUTHOR(S): Lu, Li-Bin; Zhang, Yun-Qian; Zhu, Qian-Jiang; Xue, Sai-Feng; Tao, Zhu
CORPORATE SOURCE: Institute of Applied Chemistry, Guizhou University, Guiyang, 550025, Peop. Rep. China
SOURCE: Molecules (2007), 12(4), 716-722
CODEN: MOLEFW; ISSN: 1420-3049
URL: http://www.mdpi.org/molecules/papers/12040716.pdf
PUBLISHER: Molecular Diversity Preservation International
DOCUMENT TYPE: Journal; (online computer file)
LANGUAGE: English
OTHER SOURCE(S): CASREACT 147:165907

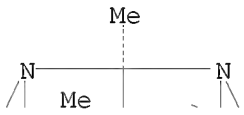
AB The synthesis, and x-ray crystal structure of the inclusion host-guest complex of dodecamethylcucurbit[6]uril (DDMeQ[6]) with 1,4-dihydroxybenzene (DHOBEN) are reported. The complex crystallizes in the space group P21/c with a = 12.2847(4), b = 12.6895(4), c = 15.1310(4) Å, α = 74.6960(10), β = 71.4090(10), γ = 86.5090(10)° and Z = 1. A novel approach to dodecamethylcucurbit[6]uril synthesis is also described. To sep. dodecamethylcucurbit[6]uril, 1,4-dihydroxybenzene is used as a guest mol. for crystallization of the fully methyl-substituted cucurbituril. The driving force for the self-assembled inclusion host-guest complex can be attributed to not only the cavity interaction of dodecamethylcucurbit[6]uril (host), but also to the hydrogen bonding between the carbonyl oxygen at the portals of the host and the hydroxy groups of the guest.

IT 569359-77-9
RL: PRP (Properties)
(preparation and X-ray structure of inclusion complex of

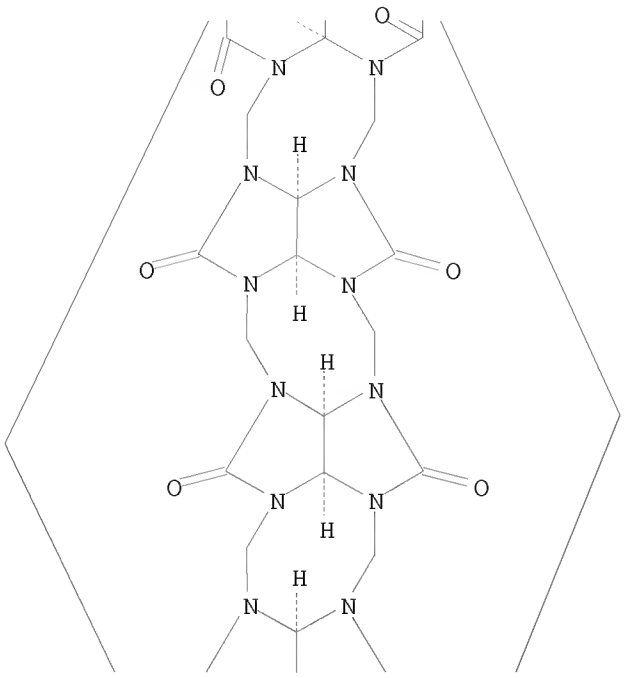
dodecamethylcucurbit[6]uril with 1,4-dihydroxybenzene)
RN 569359-77-9 CAPLUS
CN 1H,4H,12H,15H-2,14:3,13-Dimethano-
5H,6H,7H,8H,9H,10H,11H,16H,17H,18H,19H,20H,21H,22H-
2,3,4a,5a,6a,7a,8a,9a,10a,11a,13,14,15a,16a,17a,18a,19a,20a,21a,22a-
eicosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pe
ntaleno[1',6':5,6,7]cycloocta[1,2,3-cd:1',2',3'-gh]pentalene-
1,4,6,8,10,12,15,17,19,21-decone, decahydro-2a,22b-dimethyl-, stereoisomer
(CA INDEX NAME)

Relative stereochemistry.

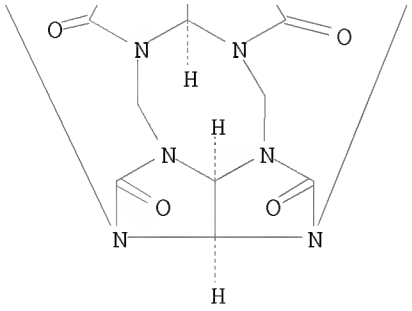
PAGE 1-A



PAGE 2-A



PAGE 3-A



REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 10 OF 18 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2007:408339 CAPLUS
DOCUMENT NUMBER: 147:52550
TITLE: Interaction between Tetramethylcucurbit[6]uril and Some Pyridine Derivates
AUTHOR(S): Cong, Hang; Tao, Long-Ling; Yu, Yi-Hua; Tao, Zhu; Yang, Fan; Zhao, Yun-Jie; Xue, Sai-Feng; Lawrance, Geoffrey A.; Wei, Gang
CORPORATE SOURCE: Institute of Applied Chemistry, Guizhou University, Guiyang, Guizhou, 550025, Peop. Rep. China

SOURCE: Journal of Physical Chemistry A (2007), 111(14), 2715-2721
CODEN: JPCAFH; ISSN: 1089-5639
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Interaction between tetramethylcucurbit[6]uril (TMeQ[6], host) with hydrochloride salts of 2-phenylpridine (G1), 2-benzylpyridine (G2), and 4-benzylpyridine (G3) (guests) have been investigated by using 1H NMR spectroscopy and electronic absorption spectroscopy and theor. calcns. The 1H NMR spectra anal. established an interaction model in which the host selectively included the Ph moiety of the HCl salt of the above three guests, and formed inclusion complexes with a host-guest ratio of 1:1. Absorption spectrophotometric anal. allowed quant. measurement of the stability of these host-guest inclusion complexes. Particularly, we have established a competitive interaction in which one host-guest inclusion complex pair is much more stable than another host-guest inclusion complex pair. The stability consts. for the three host-guest inclusion complexes of TMeQ[6]-G1, TMeQ[6]-G2, and TMeQ[6]-G3 are .apprx.2 + 106, 60.7, and 19.9 mol-1·L, resp. To understand how subtle differences in the structure of the title guests lead to a significant difference in the stability of the corresponding host-guest inclusion complexes with the TMeQ[6], ab initio theor. calcns. have been performed, not only for the gas phase but also the solution phase (water as solvent) in all cases. The calcn. results revealed that when the Ph moiety of the three pyridine derivate guests was included, the host-guest complexation reached the min., and the corresponding energy differences for the formation of the title host-guest inclusion complexes are qual. consistent with the exptl. results.

IT 848440-56-2 939823-44-6 939823-46-8
939823-48-0
RL: PRP (Properties)
(interaction between tetramethylcucurbit[6]uril and some pyridine derivates)

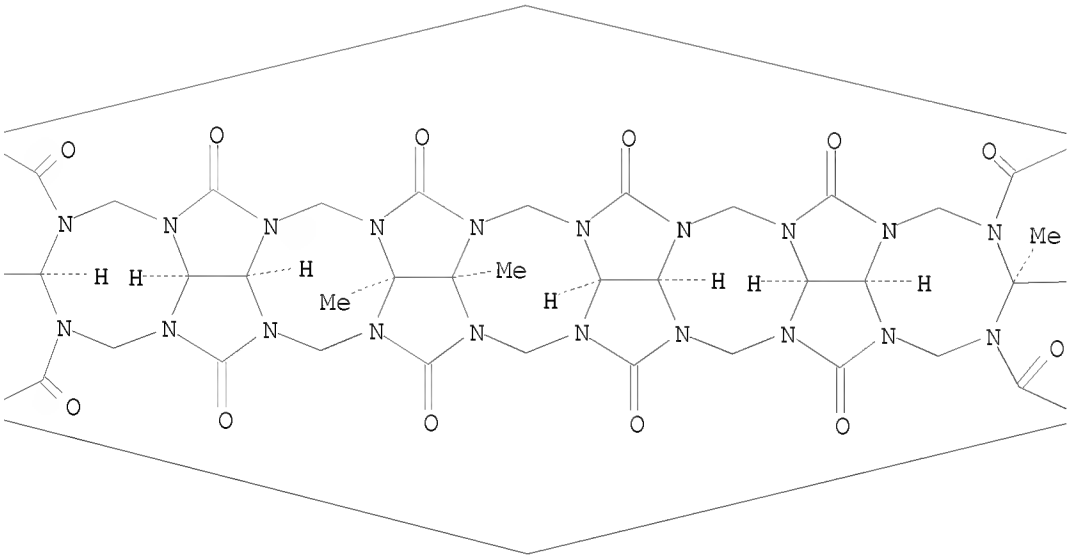
RN 848440-56-2 CAPLUS

CN 1H,4H,14H,17H-2,16:3,15-Dimethano-5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-1,4,6,8,10,12,14,17,19,21,23,25-dodecone, dodecahydro-2a,21b,21c,26b-tetramethyl-, stereoisomer (CA INDEX NAME)

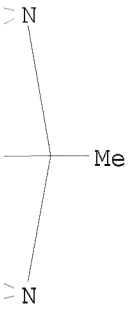
Relative stereochemistry.

PAGE 1-A

PAGE 1-B



PAGE 1-C



RN 939823-44-6 CAPLUS
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2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24
a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7''']cycloocta[1'',2''
,3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-
g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-
1,4,6,8,10,12,14,17,19,21,23,25-dodecone,
dodecahydro-2a,21b,21c,26b-tetramethyl-, stereoisomer, compd. with
2-phenylpyridine (2:5) (CA INDEX NAME)

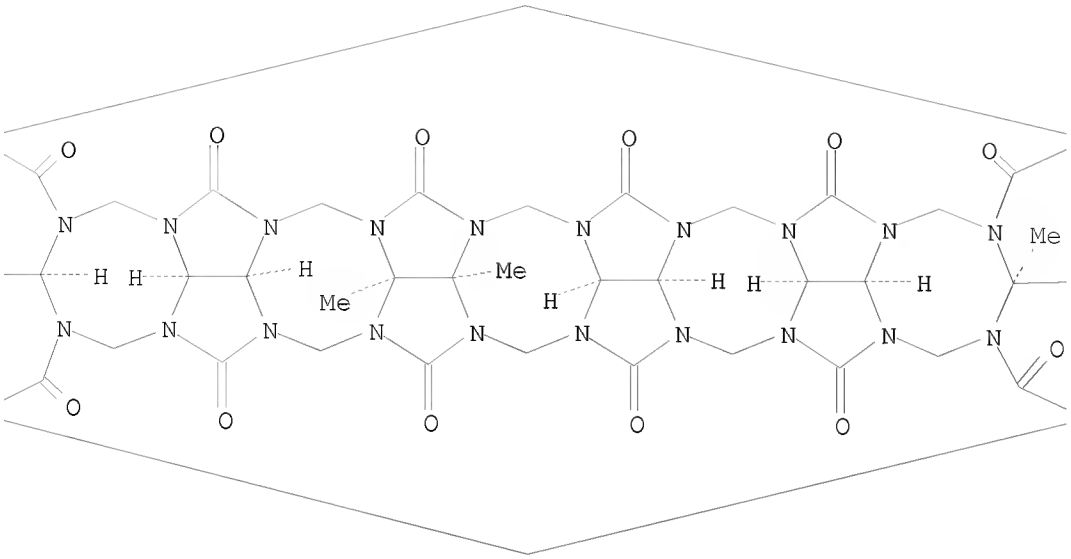
CM 1

CRN 848440-56-2
CMF C40 H44 N24 O12

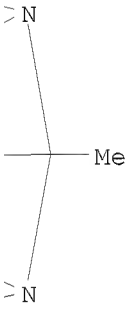
Relative stereochemistry.

PAGE 1-A

PAGE 1-B

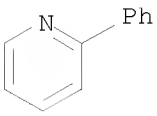


PAGE 1-C



CM 2

CRN 1008-89-5
CMF C11 H9 N



RN 939823-46-8 CAPLUS
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5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-
2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-
1,4,6,8,10,12,14,17,19,21,23,25-dodecone,
dodecahydro-2a,21b,21c,26b-tetramethyl-, stereoisomer, compd. with
2-(phenylmethyl)pyridine (2:5) (CA INDEX NAME)

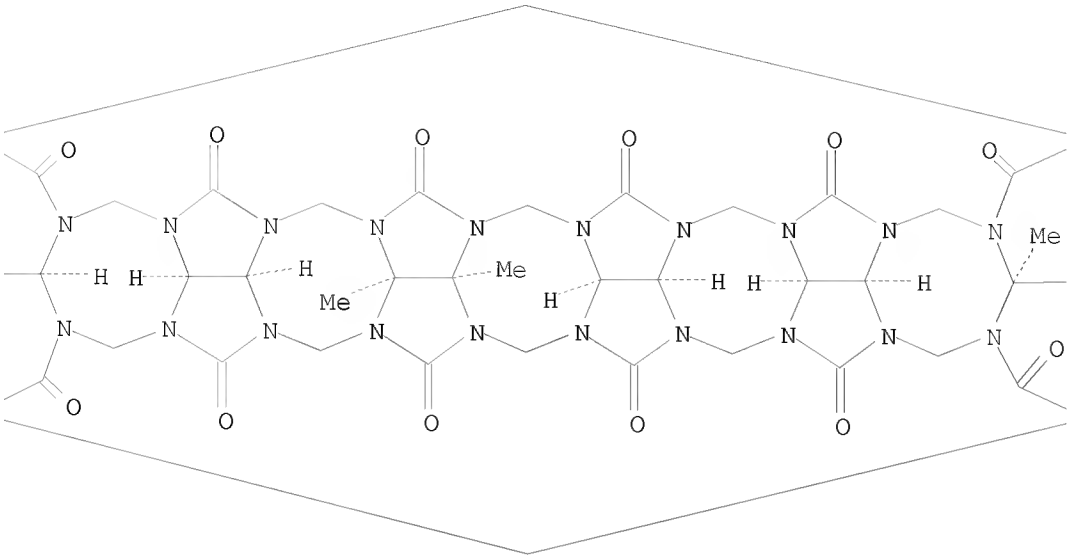
CM 1

CRN 848440-56-2
CMF C40 H44 N24 O12

Relative stereochemistry.

PAGE 1-A

PAGE 1-B



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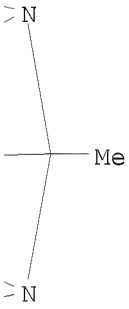
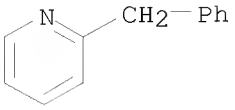


CM 2

CRN 101-82-6
CMF C12 H11 N



RN 939823-48-0 CAPLUS
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2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24
a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2''
,3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-
g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-
1,4,6,8,10,12,14,17,19,21,23,25-dodecone,
dodecahydro-2a,21b,21c,26b-tetramethyl-, stereoisomer, compd. with
4-(phenylmethyl)pyridine (2:5) (CA INDEX NAME)

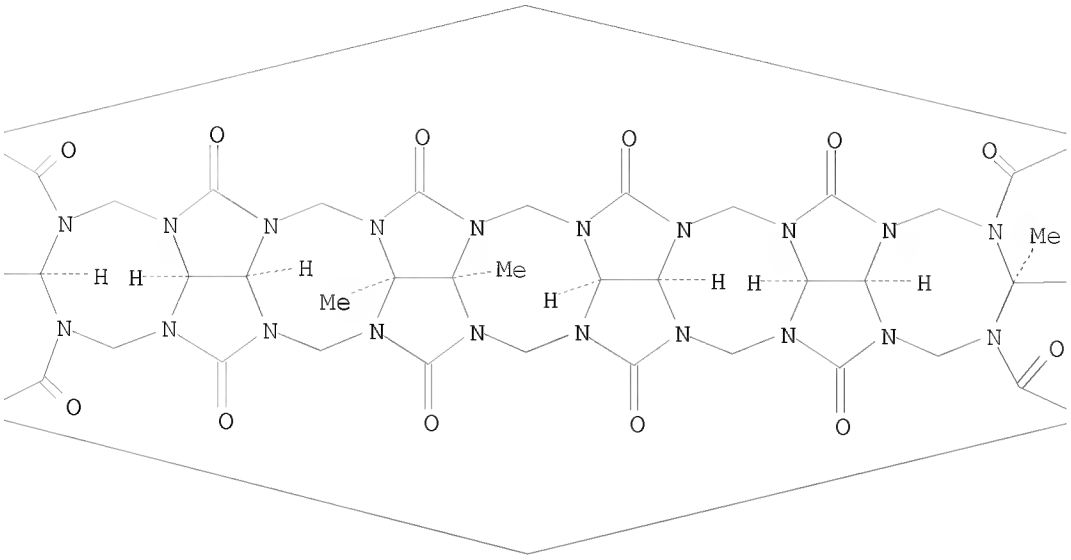
CM 1

CRN 848440-56-2
CMF C40 H44 N24 O12

Relative stereochemistry.

PAGE 1-A

PAGE 1-B



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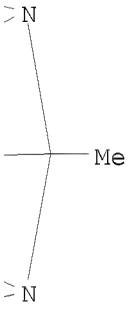
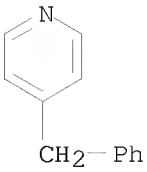


CM 2

CRN 2116-65-6
CMF C12 H11 N



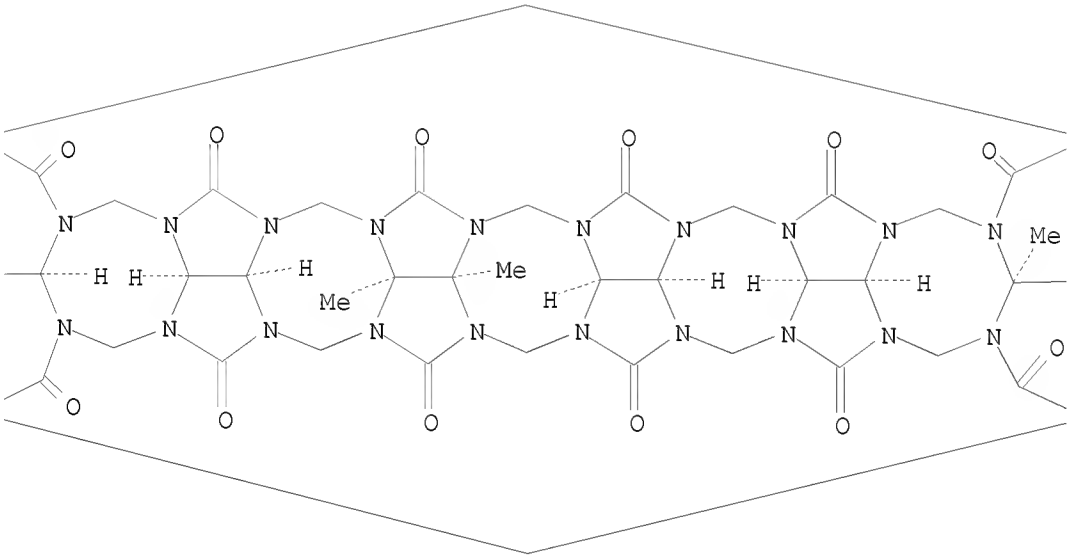
REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 11 OF 18 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2006:404036 CAPLUS
DOCUMENT NUMBER: 144:450383
TITLE: Interaction between three cucurbiturils and hydrochloride salts of 4,4'-dipyridyl and its derivates
AUTHOR(S): Mu, Lan; Xue, Sai-Feng; Du, Ying; Zhao, Yun-Jie; Zhu, Qian-Jiang; Tao, Zhu
CORPORATE SOURCE: Inst. Appl. Chem., Guizhou Univ., Guiyang, 550025, Peop. Rep. China
SOURCE: Gaodeng Xuexiao Huaxue Xuebao (2006), 27(4), 654-659
CODEN: KTHPDM; ISSN: 0251-0790
PUBLISHER: Gaodeng Jiaoyu Chubanshe
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
AB In this paper, the host-guest relationship between a general cucurbit[n = 7]uril(Q[7]) or a new ellipsoid-host - sym. tetramethyl-cucurbituril (TMeQ[6]) with hydrochloride salts of 4,4'-dipyridyl(44) or N,N'-dimethyl-4,4'-dipyridyl(dm44) was examined for confirming the interaction between cucurbituril(Q[6]) and these guests. The exptl. results revealed that Q[7] included the 4,4'-dipyridyl part of this kind of guests which were inclined in the cavity of Q[7]. The results based on 1H NMR technique, cyclic voltammetric method and UV absorption spectrophotometric measurement revealed that strong interaction existed between TMeQ[6] and guest 44 or dm44 and a one-dimensional assembled superamol. could be formed. 1H NMR technique and cyclic voltammetric method showed no obvious interaction between Q[6] with the guest 44 and its derivative, however, UV absorption spectrophotometric measurements revealed that a kind of interaction did occur; comparing the structural characteristic of Q[6] to TMeQ[6], a one-dimensional assembled superamol. could be also formed between Q[6] and guest 44 and its derivative
IT 848440-56-2
RL: PRP (Properties)
(interaction between three cucurbiturils and hydrochloride salts of 4,4'-dipyridyl and N,N'-dimethyl-4,4'-dipyridinium)
RN 848440-56-2 CAPLUS
CN 1H,4H,14H,17H-2,16:3,15-Dimethano-5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-1,4,6,8,10,12,14,17,19,21,23,25-dodecone, dodecahydro-2a,21b,21c,26b-tetramethyl-, stereoisomer (CA INDEX NAME)

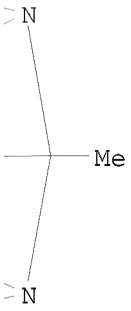
Relative stereochemistry.

PAGE 1-A

PAGE 1-B



PAGE 1-C



L4 ANSWER 12 OF 18 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:1142893 CAPLUS
DOCUMENT NUMBER: 144:323501
TITLE: Synthesis and crystal structure of a novel self-assembled 1,4-dimethyl cucurbituril silver(I) complex
AUTHOR(S): Zhang, Yun-Qian; Tao, Zhu; Zhao, Yun-Jie; Xue, Sai-Feng; Zhu, Qian-Jiang; Wei, Zhan-Bing; Long, La-Sheng
CORPORATE SOURCE: Institute of Applied Chemistry, Guizhou University, Guiyang, 550025, Peop. Rep. China
SOURCE: Wuji Huaxue Xuebao (2005), 21(10), 1576-1582
CODEN: WHUXEO; ISSN: 1001-4861
PUBLISHER: Wuji Huaxue Xuebao Bianjibu
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
OTHER SOURCE(S): CASREACT 144:323501
AB Crystals of a new 1,4-di-Me cucurbituril (TMeQ [6]) with Silver(I) ion were synthesized, and the structure was determined by X-ray diffraction technique. There are two kinds of TMeQ[6] A and B which formed mol. encapsulates with two silver ion lids in the self-assembled entities. One dimensional supramol. tubes are formed from the encapsulates A, and two dimensional mol. sieves are formed from the encapsulates B, the tubes and the sieves stack together alternately in the self-assembled entities.
IT 880076-32-4P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal structure of a novel self-assembled 1,4-di-Me cucurbituril silver(I) complex)
RN 880076-32-4 CAPLUS
CN Silver(2+), diaqua(dodecahydro-2a,21b,21c,26b-tetramethyl-1H,4H,14H,17H-2,16:3,15-dimethano-5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-1,4,6,8,10,12,14,17,19,21,23,25-dodecone)di-,

tetraaqua(dodecahydro-2a,21b,21c,26b-tetramethyl-1H,4H,14H,17H-2,16:3,15-dimethano-5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-1,4,6,8,10,12,14,17,19,21,23,25-dodecone)disilver(2+) nitrate (1:1:4), octahydrate (9CI) (CA INDEX NAME)

CM 1

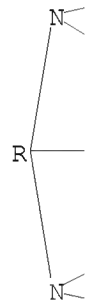
CRN 880076-31-3
CMF C40 H52 Ag2 N24 O16 . C40 H48 Ag2 N24 O14 . 4 N O3

CM 2

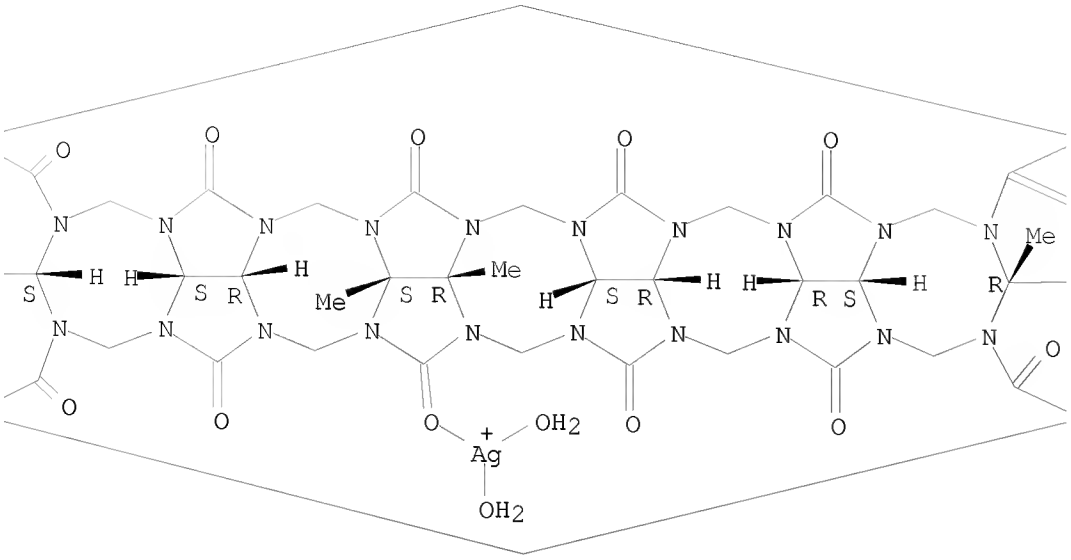
CRN 880076-30-2
CMF C40 H52 Ag2 N24 O16
CCI CCS

Relative stereochemistry.

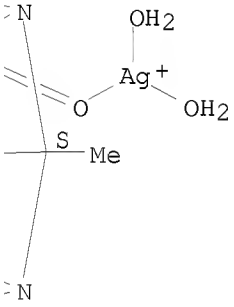
PAGE 1-A



PAGE 1-B



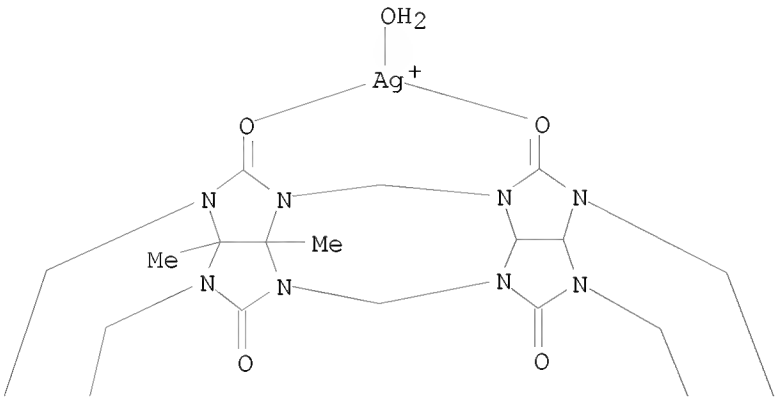
PAGE 1-C



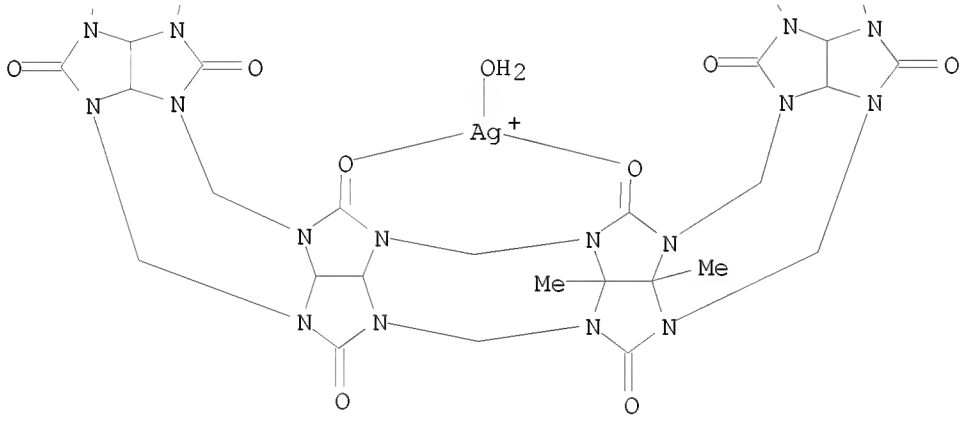
CM 3

CRN 880076-29-9
CMF C40 H48 Ag2 N24 O14
CCI CCS

PAGE 1-A

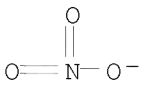


PAGE 2-A



CM 4

CRN 14797-55-8
CMF N O3

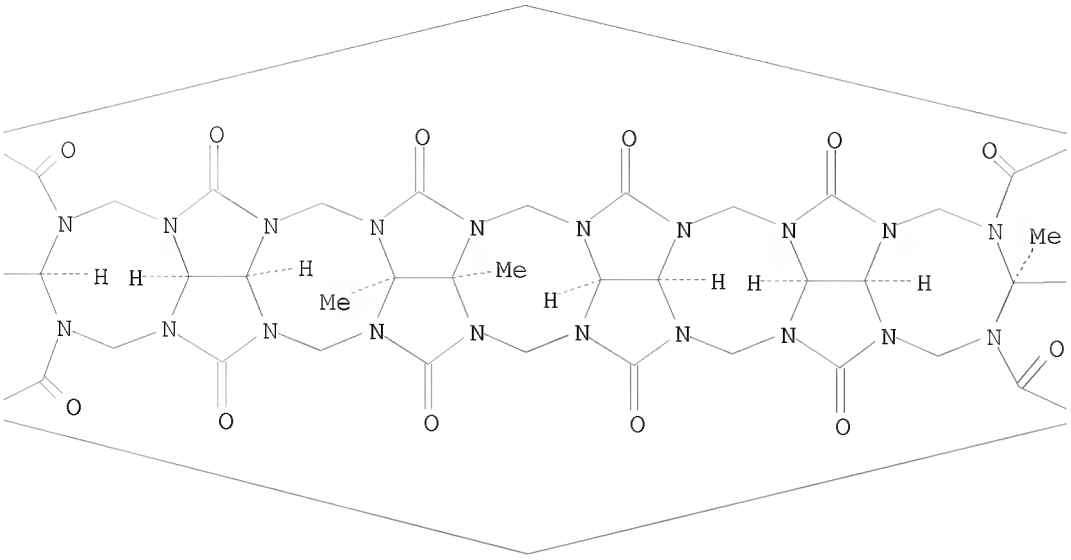


IT 848440-56-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of a novel self-assembled 1,4-di-Me cucurbituril silver(I) complex)
RN 848440-56-2 CAPLUS
CN 1H,4H,14H,17H-2,16:3,15-Dimethano-
5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-
2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-
1,4,6,8,10,12,14,17,19,21,23,25-dodecone,
dodecahydro-2a,21b,21c,26b-tetramethyl-, stereoisomer (CA INDEX NAME)

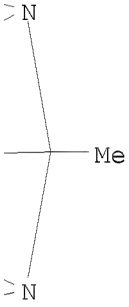
Relative stereochemistry.

PAGE 1-A

PAGE 1-B



PAGE 1-C

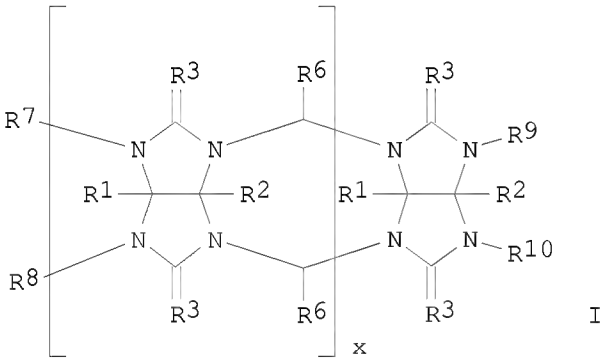


L4 ANSWER 13 OF 18 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:1042246 CAPLUS
DOCUMENT NUMBER: 143:347171
TITLE: Method for preparing compounds comprising cucurbituril groups
INVENTOR(S): Day, Anthony Ivan
PATENT ASSIGNEE(S): Unisearch Limited, Australia
SOURCE: PCT Int. Appl., 56 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent

LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2005090351	A1	20050929	WO 2005-AU396		20050318
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW					
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
AU 2005222730	A1	20050929	AU 2005-222730		20050318
CA 2556857	A1	20050929	CA 2005-2556857		20050318
EP 1725558	A1	20061129	EP 2005-714268		20050318
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR					
CN 1930169	A	20070314	CN 2005-80007986		20050318
JP 2007529428	T	20071025	JP 2007-503155		20050318
IN 2006DN04501	A	20070824	IN 2006-DN4501		20060803
KR 2006135775	A	20061229	KR 2006-717057		20060824
US 20070287836	A1	20071213	US 2007-588846		20070430
PRIORITY APPLN. INFO.:			AU 2004-901473	A	20040319
			WO 2005-AU396	W	20050318

OTHER SOURCE(S): CASREACT 143:347171; MARPAT 143:347171
GI



I

AB The present invention provides a method for preparing compds. comprising a plurality of cucurbituril groups. The method comprises forming a mixture comprising one or more compds. of the formula A-L-A wherein L is a linking group and A is group of the formula I [R1 and R2 independently = bond with L or univalent radical, or R1,R2 and the carbon atoms to which they are bound together from an (un)substituted cyclic group, or R1 of one unit and R2 of adjacent unit from a bond or divalent radical, etc.; R3 = O, S, NH,

etc.; R6 = bond with L, H, alkyl, and aryl; R7 and R8 or R9 and R10 independently = H and CHR6OR6, or R7 and R8 together form the group -CHR6OCHR6-; x = 0-10 with provisions], and an acid, and exposing the mixture to conditions effective for at least some of the groups A to form cucurbituril groups.

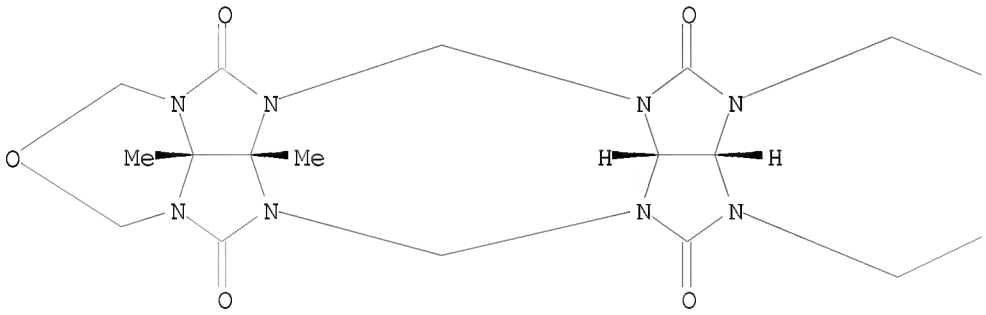
IT 865813-91-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of dimer, trimer and tetramers of glycolurils useful for preparing
compound containing plurality of cucurbituril groups)

RN 865813-91-8 CAPLUS

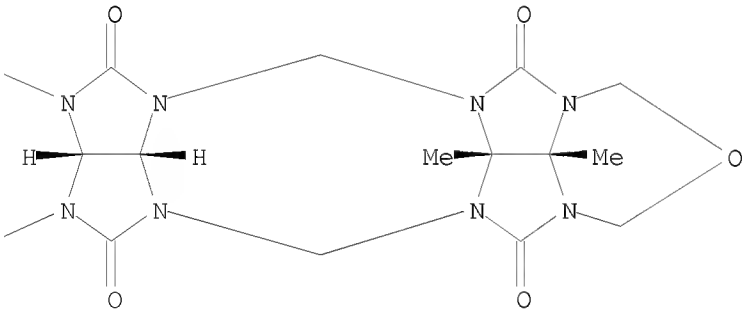
CN 1H,3H,4H,5H,6H,7H,8H,9H,10H,11H,13H,14H,15H,16H,17H,18H,19H,20H-2,12-Dioxa-3a,4a,5a,6a,7a,8a,9a,10a,13a,14a,15a,16a,17a,18a,19a,20a-hexadecaazabisbenzo[3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-4,6,8,10,14,16,18,20-octone, octahydro-, stereoisomer (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



PAGE 1-B



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 14 OF 18 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:260070 CAPLUS
DOCUMENT NUMBER: 142:336358
TITLE: Method for preparing cucurbiturils
INVENTOR(S): Day, Anthony Ivan; Arnold, Alan Peter; Blanch, Rodney

John
PATENT ASSIGNEE(S): Unisearch Limited, Australia
SOURCE: PCT Int. Appl., 58 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005026168	A1	20050324	WO 2004-AU1232	20040910
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004272121	A1	20050324	AU 2004-272121	20040910
CA 2537843	A1	20050324	CA 2004-2537843	20040910
EP 1668012	A1	20060614	EP 2004-761268	20040910
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
CN 1878774	A	20061213	CN 2004-80033392	20040910
JP 2007505046	T	20070308	JP 2006-525577	20040910
KR 2006119979	A	20061124	KR 2006-705066	20060311
US 20070066818	A1	20070322	US 2006-571707	20060313
IN 2006DN01397	A	20070803	IN 2006-DN1397	20060314
PRIORITY APPLN. INFO.:			AU 2003-905037 A	20030912
			WO 2004-AU1232 W	20040910

OTHER SOURCE(S): CASREACT 142:336358; MARPAT 142:336358

AB The invention relates to a method for preparing cucurbiturils. The method comprises reacting an oligomer consisting of 2 to 11 linked glycolurils or glycoluril analogs with one or more compds. selected from glycoluril, glycoluril analogs and/or oligomers of glycoluril or glycoluril analogs, in the presence of an acid, to form a cucurbituril. The method can be used to prepare variably substituted cucurbiturils having specific substituted units at specific locations in the cucurbituril. Thus, dimethylcucurbit[1,4]uril was obtained by treating the formaldehyde diether of dimethylglycoluril with the diether of glycoluril and paraformaldehyde in concentrated HCl.

IT 569359-77-9P 848440-55-1P 848440-56-2P
848440-58-4P 848440-61-9P 865813-91-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of cucurbiturils as complexing agents)

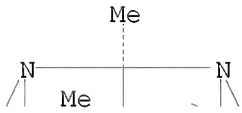
RN 569359-77-9 CAPLUS

CN 1H,4H,12H,15H-2,14:3,13-Dimethano-
5H,6H,7H,8H,9H,10H,11H,16H,17H,18H,19H,20H,21H,22H-
2,3,4a,5a,6a,7a,8a,9a,10a,11a,13,14,15a,16a,17a,18a,19a,20a,21a,22a-
eicosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-cd:1',2',3'-gh]pentalene-
1,4,6,8,10,12,15,17,19,21-decone, decahydro-2a,22b-dimethyl-, stereoisomer

(CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



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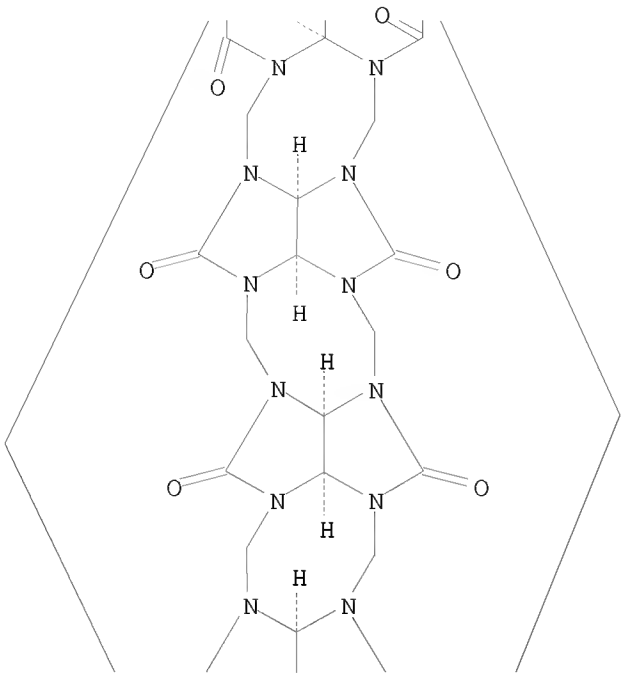
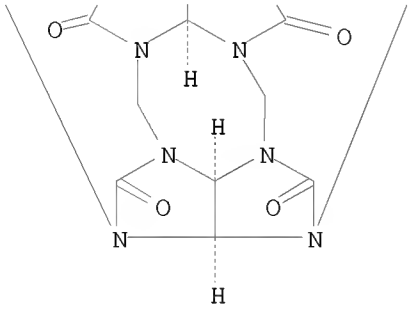
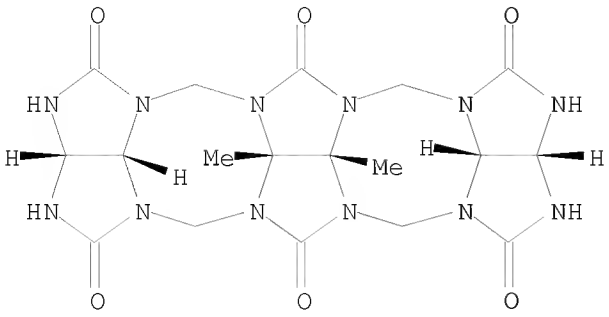


PAGE 3-A



RN 848440-55-1 CAPLUS
CN 5H,6H,7H,12H,13H,14H-2,3,4a,5a,6a,7a,9,10,11a,12a,13a,14a-Dodecaazabispentaleno[1',6':5,6,7]cycloocta[1,2,3-cd:1',2',3'-gh]pentalene-1,4,6,8,11,13(2H,3H,9H,10H)-hexone, hexahydro-13b,13c-dimethyl-, stereoisomer (9CI) (CA INDEX NAME)

Relative stereochemistry.

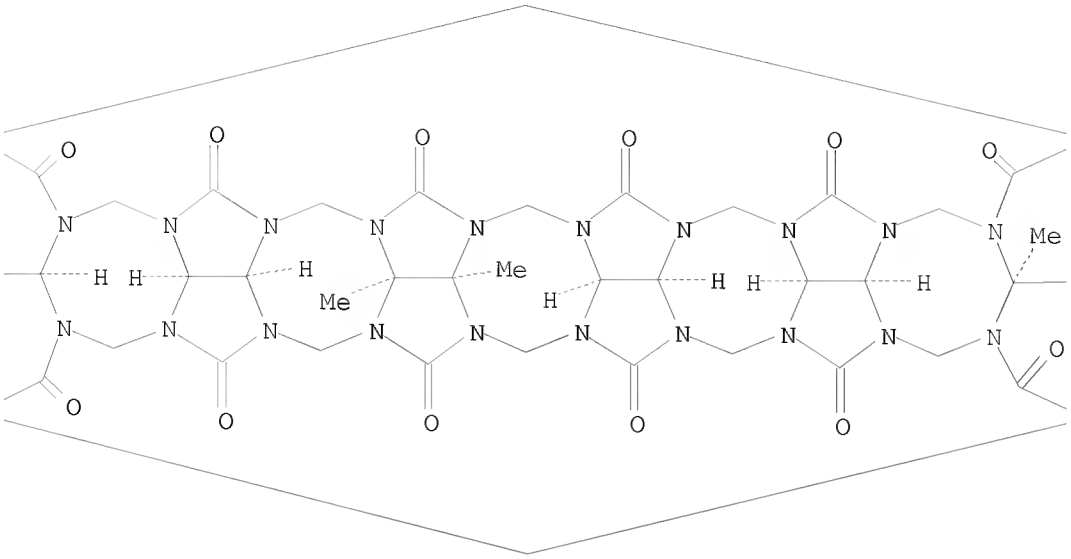


RN 848440-56-2 CAPLUS
CN 1H,4H,14H,17H-2,16:3,15-Dimethano-
5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-
2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-
1,4,6,8,10,12,14,17,19,21,23,25-dodecone,
dodecahydro-2a,21b,21c,26b-tetramethyl-, stereoisomer (CA INDEX NAME)

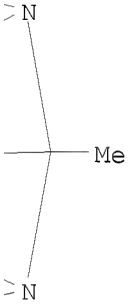
Relative stereochemistry.

PAGE 1-A

PAGE 1-B



PAGE 1-C

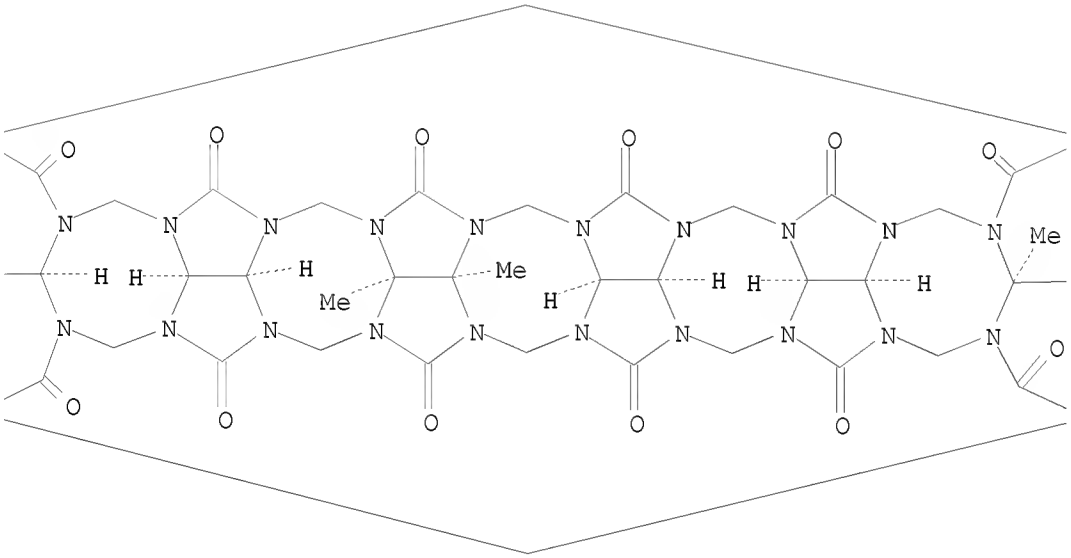


RN 848440-58-4 CAPLUS
CN 1H,4H,14H,17H-2,16:3,15-Dimethano-
5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-
2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-
1,4,6,8,10,12,14,17,19,21,23,25-dodecone,
dodecahydro-2a,21b,21c-trimethyl-26b-phenyl-, stereoisomer (9CI) (CA INDEX NAME)

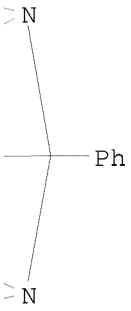
Relative stereochemistry.

PAGE 1-A

PAGE 1-B



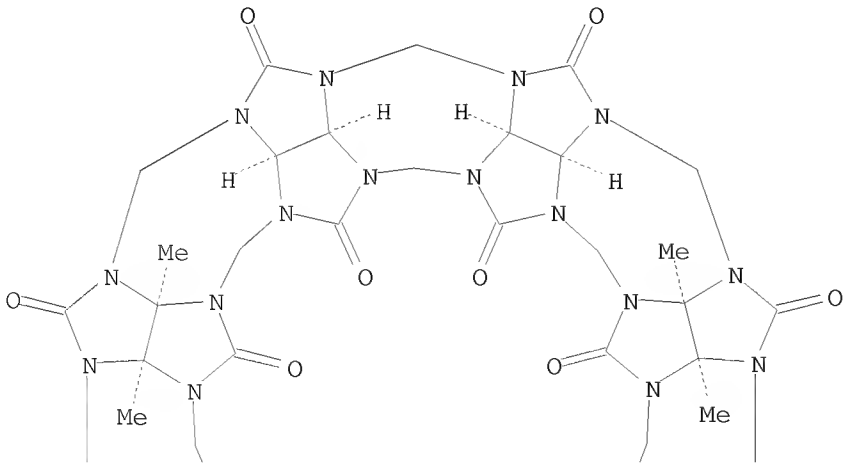
PAGE 1-C



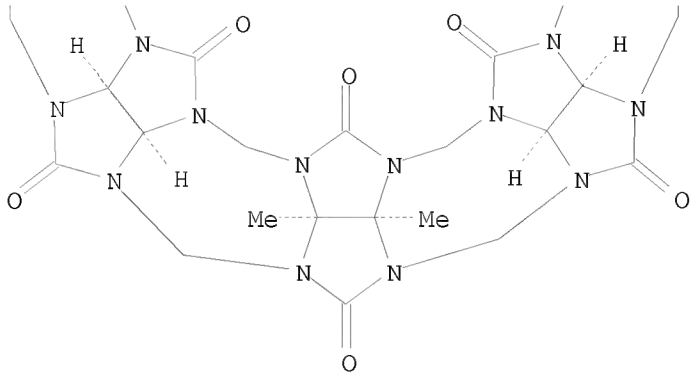
RN 848440-61-9 CAPLUS
CN 2,18:3,17-Dimethano-2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,14a,15a,17,18,19a,20a,21a,22a,23a,24a,25a,26a,27a,28a,29a,30a-octacosaazabispentaleno[1''''',6''''':5'''',6'''',7''''']cycloocta[1'''',2''',3'''':3''',4''']pentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-cd:1',2',3'-gh]pentalene-1,4,6,8,10,12,14,16,19,21,23,25,27,29-tetradecone, tetradecahydro-2a,21b,21c,25b,25c,30b-hexamethyl-, stereoisomer (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



PAGE 2-A

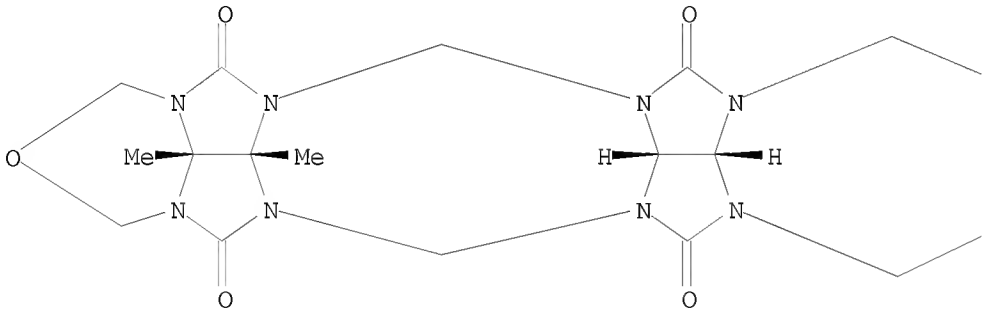


RN 865813-91-8 CAPLUS

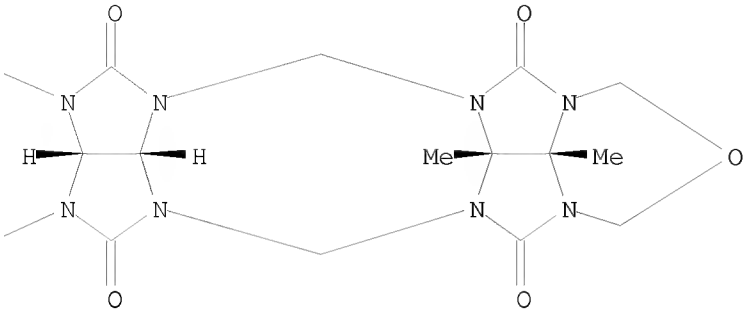
CN 1H,3H,4H,5H,6H,7H,8H,9H,10H,11H,13H,14H,15H,16H,17H,18H,19H,20H-2,12-Dioxa-3a,4a,5a,6a,7a,8a,9a,10a,13a,14a,15a,16a,17a,18a,19a,20a-hexadecaazabisbenzo[3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-4,6,8,10,14,16,18,20-octone, octahydro-, stereoisomer (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



PAGE 1-B



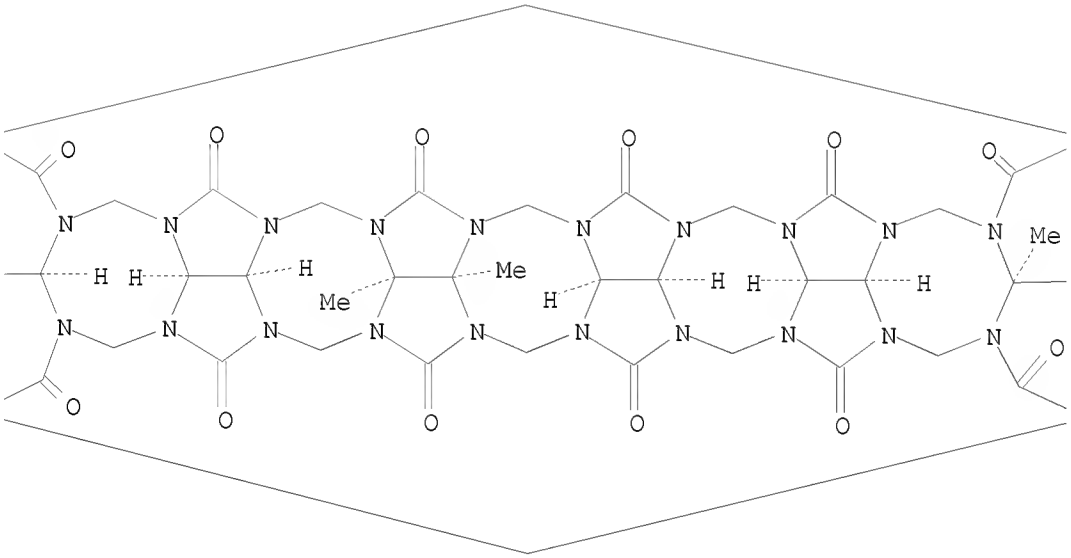
REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 15 OF 18 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2004:684964 CAPLUS
DOCUMENT NUMBER: 143:7687
TITLE: Synthesis of a symmetrical tetrasubstituted cucurbit[6]uril and its host-guest inclusion complex with 2,2'-bipyridine
AUTHOR(S): Zhao, Yunjie; Xue, Saifeng; Zhu, Qianjiang; Tao, Zhu; Zhang, Jianxin; Wei, Zhanbin; Long, Lasheng; Hu, Maolin; Xiao, Hongping; Day, Anthony I.
CORPORATE SOURCE: Institute of Applied Chemistry, Guizhou University, Guiyang, 550025, Peop. Rep. China
SOURCE: Chinese Science Bulletin (2004), 49(11), 1111-1116
CODEN: CSBUEF; ISSN: 1001-6538
PUBLISHER: Science in China Press
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 143:7687
AB Synthesis of a sym. tetramethylcucurbit[6]uril (TMeQ[6]) has been achieved by using the diether of dimethylglycoluril and the dimer of glycoluril. The structure of TMeQ[6] has been determined by single crystal X-ray diffraction, 1H NMR spectroscopy and ESMS. The 1H NMR spectra of 2,2'-bipyridine added to TMeQ[6] reveal that the host-guest inclusion complex was easily formed.
IT 848440-56-2P
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(preparation and crystal structure of sym. tetrasubstituted cucurbit[6]uril and its host-guest inclusion complex with bipyridine)
RN 848440-56-2 CAPLUS
CN 1H,4H,14H,17H-2,16:3,15-Dimethano-5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-1,4,6,8,10,12,14,17,19,21,23,25-dodecone, dodecahydro-2a,21b,21c,26b-tetramethyl-, stereoisomer (CA INDEX NAME)

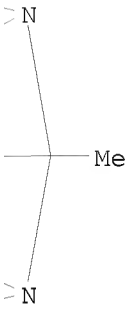
Relative stereochemistry.

PAGE 1-A

PAGE 1-B



PAGE 1-C



REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 16 OF 18 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2003:590408 CAPLUS
DOCUMENT NUMBER: 139:135453
TITLE: Cucurbiturils and method for binding gases and volatiles using cucurbiturils
INVENTOR(S): Day, Anthony Ivan; Arnold, Alan Peter; Blanch, Rodney John
PATENT ASSIGNEE(S): Unisearch Limited, Australia
SOURCE: U.S. Pat. Appl. Publ., 12 pp., Cont.-in-part of U. S. Ser. No. 999,770.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20030140787	A1	20030731	US 2002-301874	20021122
US 6869466	B2	20050322		
WO 2000068232	A1	20001116	WO 2000-AU412	20000505
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6793839	B1	20040921	US 2002-959770	20020107
AU 2002302117	A1	20030320	AU 2002-302117	20021122
AU 2002302117	B2	20060810		
IN 2006DE02152	A	20070907	IN 2006-DE2152	20060928
PRIORITY APPLN. INFO.:			AU 1999-232 A	19990507

WO 2000-AU412	W	20000505
AU 2001-9031	A	20011122
US 2002-959770	A2	20020107
AU 2000-43851	A	20000505
IN 2000-DE485	A3	20000508

AB Gases or volatile compds. are bound by cucurbiturils as a cucurbituril-gas/volatile complex. The gases or volatile compds. can be separated from a mixture of compds. by contacting the mix with a cucurbituril whereby at least some of the gas or volatile compound is bound to the cucurbituril to form a cucurbituril complex, followed by the release of at least some of the bound gas or volatile compound from that complex. The use of cucurbiturils in binding gases and volatile compds. is suitable for storage, safety, delivery or other uses, such as the trapping of an unpleasant or toxic gas or volatile compound

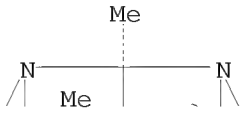
IT 569359-77-9 569363-90-2 569363-91-3
RL: TEM (Technical or engineered material use); USES (Uses)
(cucurbiturils and method for binding gases and volatiles using cucurbiturils)

RN 569359-77-9 CAPLUS

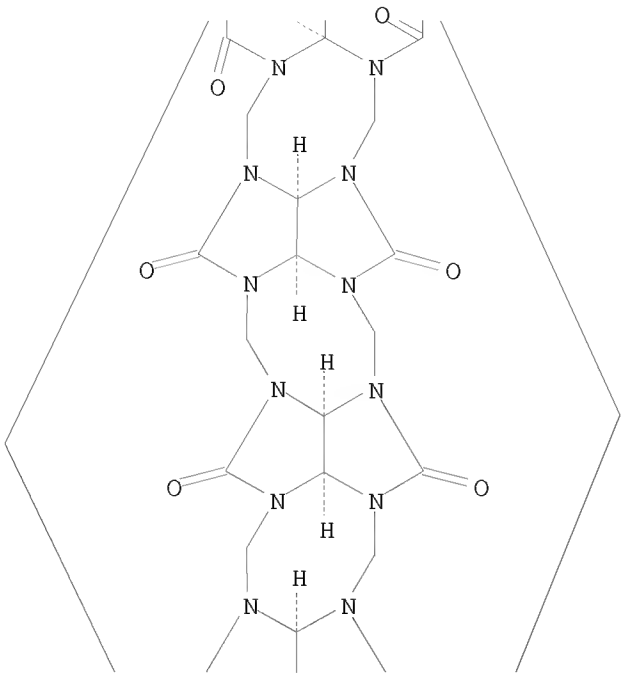
CN 1H,4H,12H,15H-2,14:3,13-Dimethano-
5H,6H,7H,8H,9H,10H,11H,16H,17H,18H,19H,20H,21H,22H-
2,3,4a,5a,6a,7a,8a,9a,10a,11a,13,14,15a,16a,17a,18a,19a,20a,21a,22a-
eicosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-cd:1',2',3'-gh]pentalene-
1,4,6,8,10,12,15,17,19,21-decone, decahydro-2a,22b-dimethyl-, stereoisomer
(CA INDEX NAME)

Relative stereochemistry.

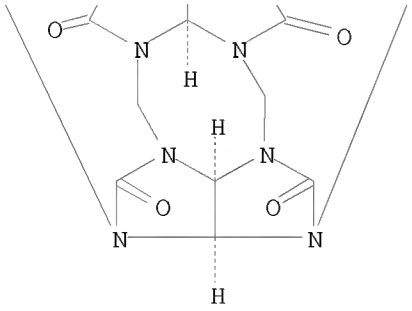
PAGE 1-A



PAGE 2-A

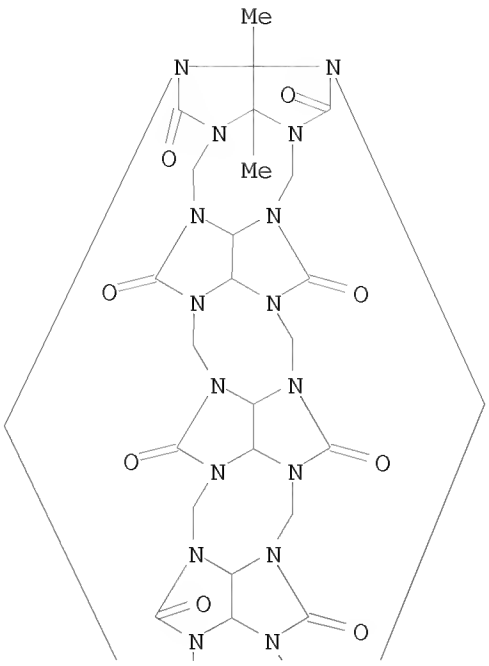


PAGE 3-A

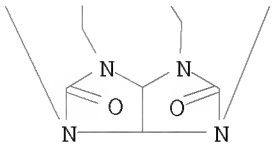


RN 569363-90-2 CAPLUS
CN 1H,4H,12H,15H-2,14:3,13-Dimethano-
5H,6H,7H,8H,9H,10H,11H,16H,17H,18H,19H,20H,21H,22H-
2,3,4a,5a,6a,7a,8a,9a,10a,11a,13,14,15a,16a,17a,18a,19a,20a,21a,22a-
eicosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pe
ntaleno[1',6':5,6,7]cycloocta[1,2,3-cd:1',2',3'-gh]pentalene-
1,4,6,8,10,12,15,17,19,21-decone, decahydro-2a,13a,15b,22b(or
2a,17b,17c,22b)-tetramethyl-, stereoisomer (9CI) (CA INDEX NAME)

PAGE 1-A

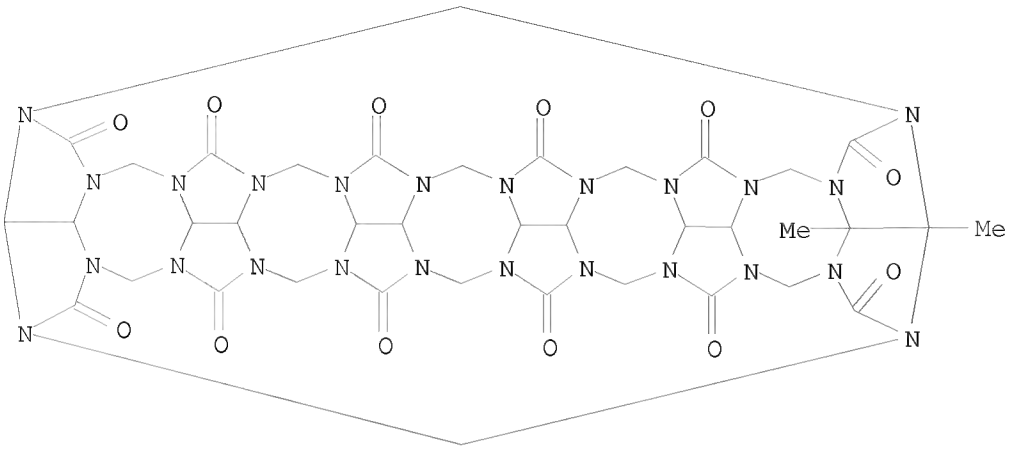


PAGE 2-A



2 (D1—Me)

RN 569363-91-3 CAPLUS
CN 1H,4H,14H,17H-2,16:3,15-Dimethano-
5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-
2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24
a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7''']cycloocta[1'',2''
,3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-
g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-
1,4,6,8,10,12,14,17,19,21,23,25-dodecone,
dodecahydro-2a,26b,?,?,?,?-hexamethyl-, stereoisomer (9CI) (CA INDEX
NAME)



4 (D1—Me)

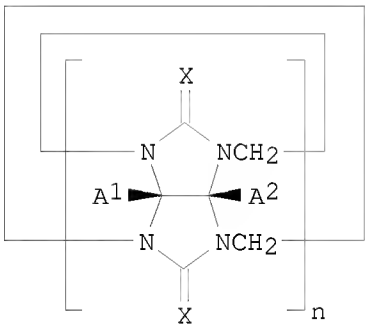
L4 ANSWER 17 OF 18 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2003:532669 CAPLUS
DOCUMENT NUMBER: 139:101129
TITLE: Methods for preparation of hydroxycucurbituril derivatives and their uses
INVENTOR(S): Kim, Ki-Moon; Jon, Sang-Yong; Selvapalam, Narayanan; Oh, Dong-Hyun
PATENT ASSIGNEE(S): Postech Foundation, S. Korea
SOURCE: PCT Int. Appl., 45 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003055888	A1	20030710	WO 2002-KR2213	20021126
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
KR 2003060053	A	20030712	KR 2002-68362	20021106
CA 2468801	A1	20030710	CA 2002-2468801	20021126
AU 2002361511	A1	20030715	AU 2002-361511	20021126
AU 2002361511	B2	20061005		
EP 1463732	A1	20041006	EP 2002-796981	20021126

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK						
CN 1604899	A	20050406	CN 2002-825227			20021126
JP 2005526708	T	20050908	JP 2003-556418			20021126
NZ 533179	A	20060331	NZ 2002-533179			20021126
IN 2004DN01493	A	20070316	IN 2004-DN1493			20040601
US 20050075498	A1	20050407	US 2004-497464			20040602
US 7388099	B2	20080617				
US 20080260676	A1	20081023	US 2008-138883			20080613
PRIORITY APPLN. INFO.:			KR 2002-318		A	20020103
			KR 2002-68362		A	20021106
			KR 2002-2002		A	20020103
			WO 2002-KR2213		W	20021126
			US 2004-497464		A3	20040602

OTHER SOURCE(S): CASREACT 139:101129; MARPAT 139:101129

GI



I

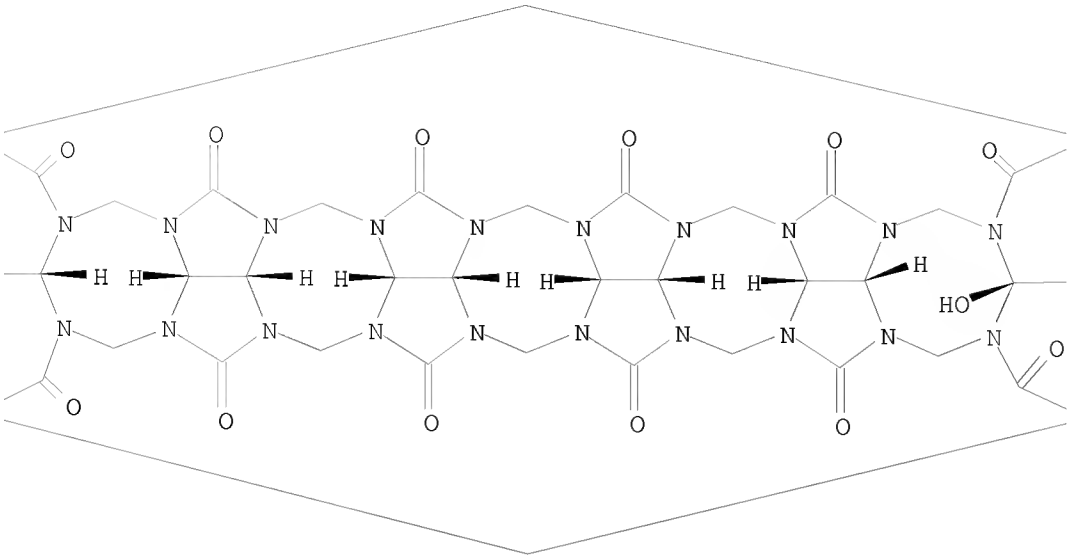
AB Provided are hydroxycucurbituril derivs., e.g., I [A1, A2 = OH, (un)substituted C1-30-alkoxy, C1-30-alkenyloxy (sic), C1-30-alkynyloxy (sic), C2-30-carbonylalkoxy, C1-30-thioalkoxy, C1-30-alkylthioloxy, C1-30-hydroxyalkoxy, C1-30-alkylsilyloxy, C1-30-aminoalkoxy, C1-30-aminoalkylthioalkoxy, C5-30-cycloalkoxy, C2-30-heterocycloalkoxy, C6-30-aryloxy, C6-20-arylalkoxy, C4-30-heteroaryloxy , C1-30-alkylthio, C1-30-alkenylthio (sic), C1-30-alkynylthio (sic), C2-30-carbonylalkylthio, C1-30-alkylsilylthio, C1-30-aminoalkylthio, C1-30-aminoalkylthioalkylthio, C5-30-cycloalkylthio, C2-30-heterocycloalkylthio, C6-30-arylthio, C6-20-arylalkylthio (sic), C4-30-heteroarylthio, C4-30-heteroarylalkylthio, C1-30-alkylamino, C1-30-alkenylamino (sic), C1-30-alkynylamino (sic), C2-30-carbonylalkylamino, C1-30-thioalkylamino, C1-30-hydroxyalkylamino, C1-30-alkylsilylamino, C1-30-aminoalkylamino, C5-30-cycloalkylamino, C2-30-heterocycloalkylamino, C6-30-arylamino, C4-30-heteroarylamino; A1 = A2 = H; X = O, S, NH; n = 4 - 20], their preparation methods and uses. Thus, hydroxycucurbit[6]uril (I; A1 = A2 = OH, X = O, n = 6) was prepared in 55% yield from cucurbit[6]uril (I; A1 = A2 = H, X = O, n = 6) via oxidation with aqueous K2S2O8. The hydroxycucurbituril derivative is easy to further functionalize with enhanced solubility in common solvents, thereby providing wider applications, e.g., in agrochems., cosmetics, medicinals and wastewater treatment. Hydroxycucurbit[6]uril formed: a 1:1 host-guest complex with THF; a 1:1 host-guest complex with isobutene; and formed an ion selective membrane with polyvinyl chloride.

IT 558445-98-0P
RL: AMX (Analytical matrix); BSU (Biological study, unclassified); MOA (Modifier or additive use); REM (Removal or disposal); SPN (Synthetic preparation); TEM (Technical or engineered material use); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(preparation of hydroxycucurbituril derivs. and their uses)
RN 558445-98-0 CAPLUS
CN 1H,4H,14H,17H-2,16:3,15-Dimethano-
5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-
2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-
1,4,6,8,10,12,14,17,19,21,23,25-dodecone, dodecahydro-2a,26b-dihydroxy-, stereoisomer (9CI) (CA INDEX NAME)

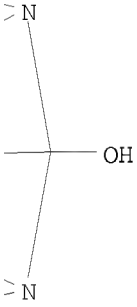
Relative stereochemistry.

PAGE 1-A

PAGE 1-B



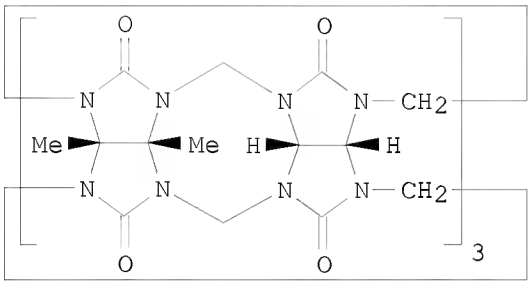
PAGE 1-C



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 18 OF 18 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2003:316145 CAPLUS
DOCUMENT NUMBER: 140:77122
TITLE: A method for synthesizing partially substituted cucurbit[n]uril
AUTHOR(S): Day, Anthony I.; Arnold, Alan P.; Blanch, Rodney J.
CORPORATE SOURCE: School of Chemistry, University College (UNSW), Australian Defence Force Academy, Canberra, ACT 2600,

Australia
SOURCE: Molecules (2003), 8(1), 74-84
CODEN: MOLEFW; ISSN: 1420-3049
URL: http://www.mdpi.org/molecules/papers/80100074.pdf
PUBLISHER: Molecular Diversity Preservation International
DOCUMENT TYPE: Journal; (online computer file)
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:77122
GI



I

AB A novel approach to cucurbituril synthesis is described where partial substitution is introduced into cucurbit[n]uril. The identification of homologs (and their substitution) in reaction mixts. is achieved by a combination of ESMS and the use of the mol. probes (guests) 1,4-dioxane and 1,9-octanediamine. A unique sym. hexamethylcucurbit[3,3]uril (I), the major product, was isolated and characterized.

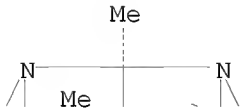
IT 569359-77-9P 640732-36-1P 640732-37-2P
640732-38-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(cyclocondensation of glycouril and its dimethyltetracyclic ether in preparation of partially substituted cucurbituril cyclic oligomers)

RN 569359-77-9 CAPLUS

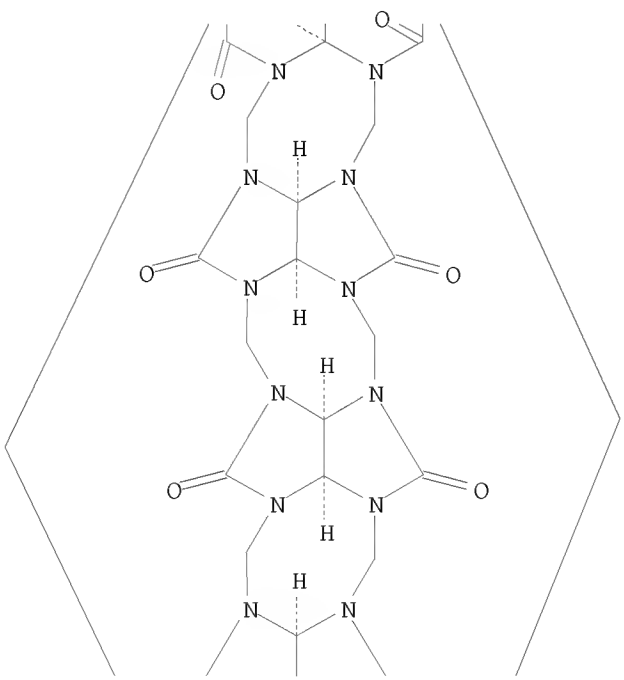
CN 1H,4H,12H,15H-2,14:3,13-Dimethano-
5H,6H,7H,8H,9H,10H,11H,16H,17H,18H,19H,20H,21H,22H-
2,3,4a,5a,6a,7a,8a,9a,10a,11a,13,14,15a,16a,17a,18a,19a,20a,21a,22a-
eicosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-cd:1',2',3'-gh]pentalene-
1,4,6,8,10,12,15,17,19,21-decone, decahydro-2a,22b-dimethyl-, stereoisomer
(CA INDEX NAME)

Relative stereochemistry.

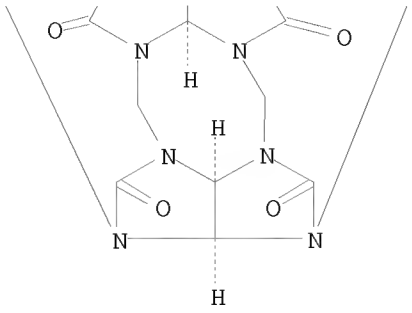
PAGE 1-A



PAGE 2-A



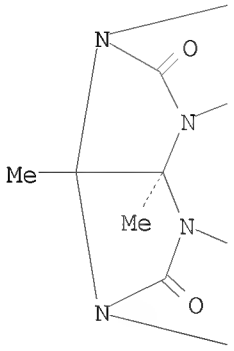
PAGE 3-A



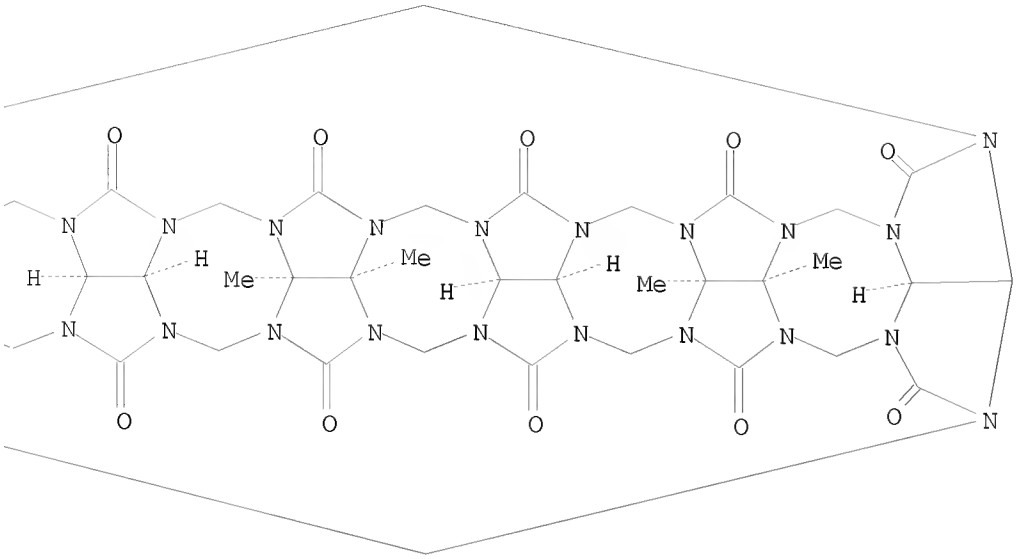
RN 640732-36-1 CAPLUS
CN 1H,4H,14H,17H-2,16:3,15-Dimethano-
5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-
2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-
1,4,6,8,10,12,14,17,19,21,23,25-dodecone,
dodecahydro-2a,19b,19c,23b,23c,26b-hexamethyl-, stereoisomer (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



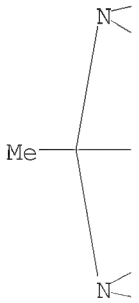
PAGE 1-B



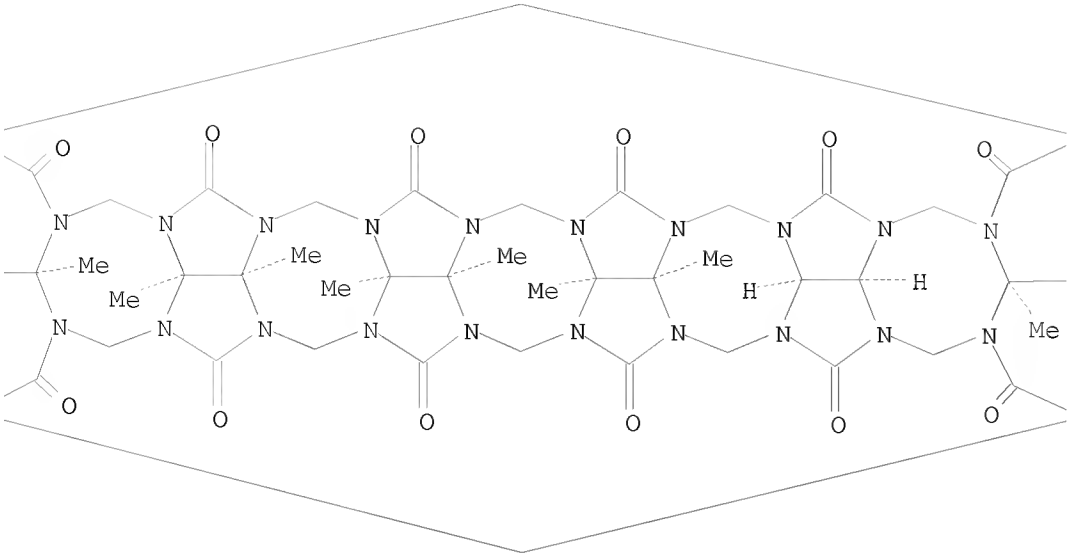
RN 640732-37-2 CAPLUS
CN 1H,4H,14H,17H-2,16:3,15-Dimethano-
5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-
2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-
1,4,6,8,10,12,14,17,19,21,23,25-dodecone,
dodecahydro-2a,15a,17b,19b,19c,21b,21c,23b,23c,26b-decamethyl-,
stereoisomer (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



PAGE 1-B



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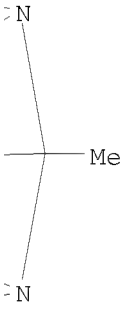
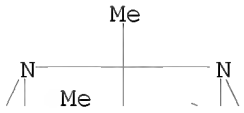
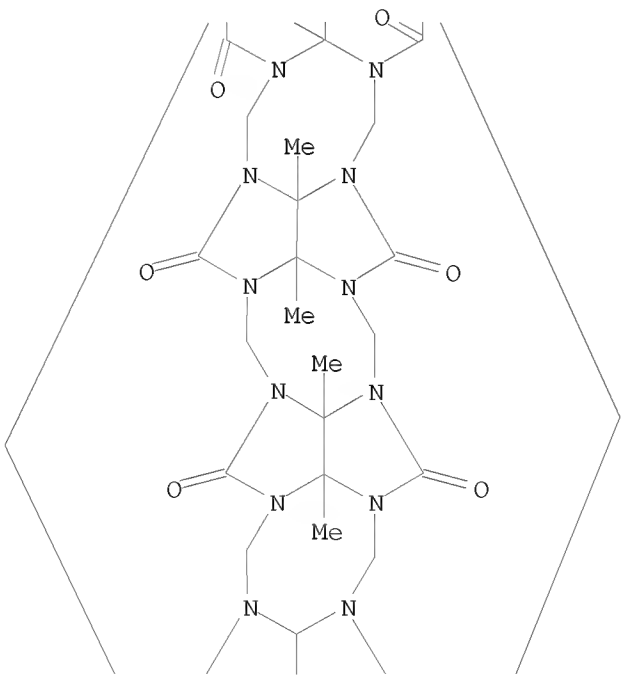


RN 640732-38-3 CAPLUS
CN 1H,4H,12H,15H-2,14:3,13-Dimethano-
5H,6H,7H,8H,9H,10H,11H,16H,17H,18H,19H,20H,21H,22H-
2,3,4a,5a,6a,7a,8a,9a,10a,11a,13,14,15a,16a,17a,18a,19a,20a,21a,22a-
eicosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pe
ntaleno[1',6':5,6,7]cycloocta[1,2,3-cd:1',2',3'-gh]pentalene-
1,4,6,8,10,12,15,17,19,21-decone, decahydro-2a,13a,15b,17b,17c,19b,19c,22b-
octamethyl-, stereoisomer (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



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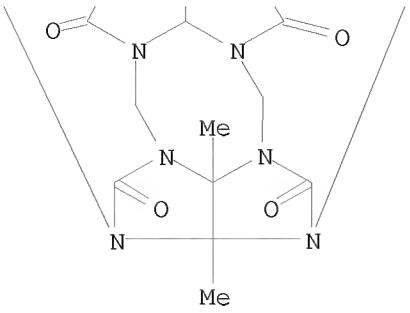

REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
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